



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:27 AM UTC

PDB ID : 8YVF / pdb_00008yvf
EMDB ID : EMD-39599
Title : cryo-EM structure of carboxysomal midi-shell: assembly from CsoS4A/4B/1A/1B/1C/1D and CsoS2 C-terminal co-expression (T=9 Q=12)
Authors : Wang, P.; Li, J.X.; Li, T.P.; Li, K.; Ng, P.C.; Wang, S.M.; Chriscoli, V.; Basle, A.; Marles-Wright, J.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2024-03-28
Resolution : 2.99 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:

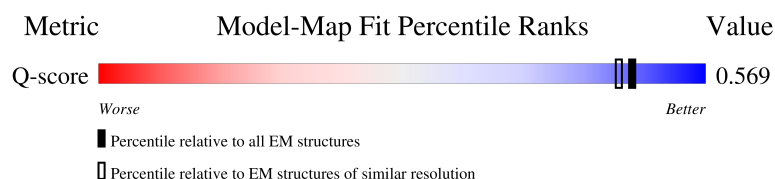
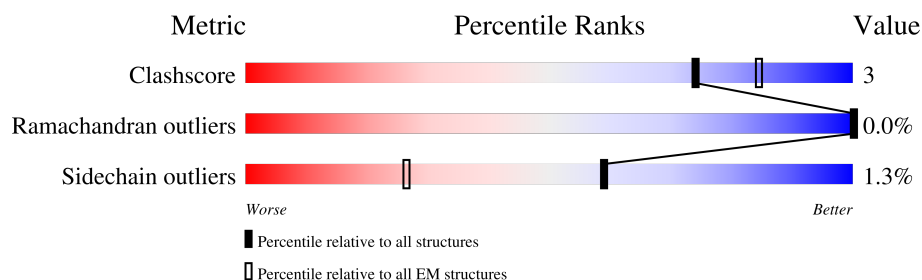
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.99 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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13287 (2.49 - 3.49)

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	0	98	
1	2	98	
1	3	98	
1	5	98	

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Mol	Chain	Length	Quality of chain
1	6	98	
1	7	98	
1	8	98	
1	9	98	
1	A	98	
1	A1	98	
1	B	98	
1	C	98	
1	D	98	
1	E	98	
1	F	98	
1	G	98	
1	H	98	
1	I	98	
1	J	98	
1	K	98	
1	L	98	
1	M	98	
1	N	98	
1	O	98	
1	P	98	
1	Q	98	
1	R	98	
1	S	98	
1	T	98	

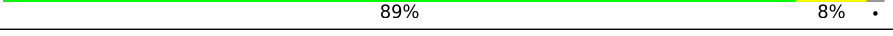
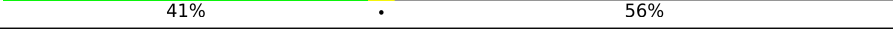
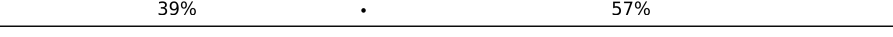
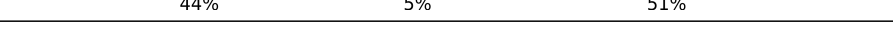
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Mol	Chain	Length	Quality of chain
1	U	98	
1	V	98	
1	W	98	
1	X	98	
1	Y	98	
1	Z	98	
1	a	98	
1	b	98	
1	c	98	
1	d	98	
1	e	98	
1	f	98	
1	g	98	
1	h	98	
1	i	98	
1	j	98	
1	k	98	
1	l	98	
1	m	98	
1	n	98	
1	o	98	
1	p	98	
1	q	98	
1	r	98	
1	s	98	

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Mol	Chain	Length	Quality of chain
1	t	98	 88% 6% 6%
1	u	98	 86% 8% 6%
1	v	98	 86% 8% 6%
2	1	83	 88% 10% .
2	4	83	 90% 7% .
2	w	83	 77% 19% ..
2	x	83	 90% 7% .
2	y	83	 84% 13% .
2	z	83	 89% 8% .
3	A2	279	 41% . 56%
3	A3	279	 39% . 57%
3	A4	279	 38% . 59%
3	A5	279	 37% 5% 58%
3	A6	279	 44% 5% 51%
3	A7	279	 35% 6% 58%
3	X1	279	 15% . 83%
3	X2	279	 14% . 83%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 47066 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 Major carboxysome shell protein CsoS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	2	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	3	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	5	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	6	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	7	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	8	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	9	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	B	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	C	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	P	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Q	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	R	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	S	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	T	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	U	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	V	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	W	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	X	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Y	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Z	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	a	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	b	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	c	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	d	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	e	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	f	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	g	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	h	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	i	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	j	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	k	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	l	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	m	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	n	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	o	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	p	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	q	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	r	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	s	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	t	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	u	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	v	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A1	92	Total 656	C 408	N 123	O 122	S 3	0	0

- Molecule 2 is a protein called Carboxysome shell vertex protein CsoS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	4	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	w	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	x	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	y	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	z	81	Total	C	N	O	S	0	0
			608	386	105	112	5		

- Molecule 3 is a protein called Carboxysome assembly protein CsoS2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	123	Total	C	N	O	S	0	0
			908	546	178	179	5		
3	A3	120	Total	C	N	O	S	0	0
			884	534	171	174	5		
3	A4	115	Total	C	N	O	S	0	0
			842	506	162	169	5		
3	A5	118	Total	C	N	O	S	0	0
			862	519	166	172	5		
3	A6	136	Total	C	N	O	S	0	0
			1000	602	196	197	5		
3	A7	117	Total	C	N	O	S	0	0
			856	517	164	171	4		
3	X1	48	Total	C	N	O	S	0	0
			337	199	55	81	2		
3	X2	48	Total	C	N	O	S	0	0
			337	199	55	81	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	591	MET	-	initiating methionine	UNP O85041
A3	591	MET	-	initiating methionine	UNP O85041
A4	591	MET	-	initiating methionine	UNP O85041
A5	591	MET	-	initiating methionine	UNP O85041
A6	591	MET	-	initiating methionine	UNP O85041
A7	591	MET	-	initiating methionine	UNP O85041
X1	591	MET	-	initiating methionine	UNP O85041
X2	591	MET	-	initiating methionine	UNP O85041

3 Residue-property plots [i](#)

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

- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 0: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 2: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 3: 



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 5: 



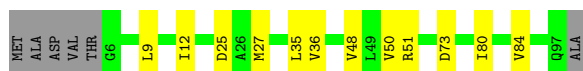
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 6: 



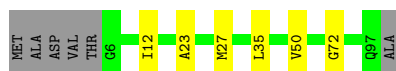
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 7:  82% 12% 6%



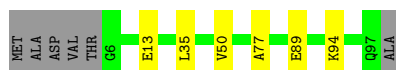
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 8:  88% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 9:  88% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain B:  87% 7% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain C:  83% 11% 6%



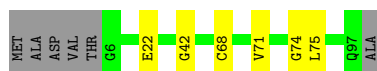
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain D:  90% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain E:  88% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain F:  93% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain G:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain H:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain I:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L:  89% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain N:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain O:  87% 7% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain P:  88% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Q:  91% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain R:  89% 5% 6%



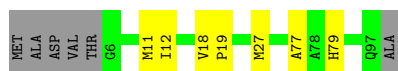
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain S:  91% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain T:  87% 7% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain U:  80% 14% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain V:  85% 9% 6%



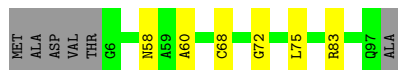
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain W:  79% 15% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain X:  88% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Y:  82% 12% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Z:  90% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain a:  85% 8% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain b:  81% 13% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain c:  89% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain d:  84% 10% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain e:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain f:  91% • 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain g:  83% 11% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain h:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain i:  83% 11% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain j:  89% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain k:  81% 12% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain l:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain m:  89% 5% 6%



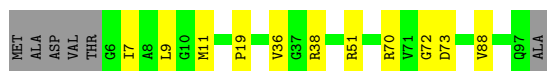
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain n:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain o:  83% 11% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain p:  89% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain q:  87% 7% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain r:  88% 5% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain s:  90% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain t:  88% 6% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain u:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain v:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain A1:  87% 6% 6%



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain 1:  88% 10% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain 4:  90% 7% .



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain w:  77% 19% ..



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain x:  90% 7% .

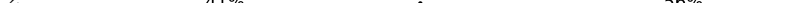


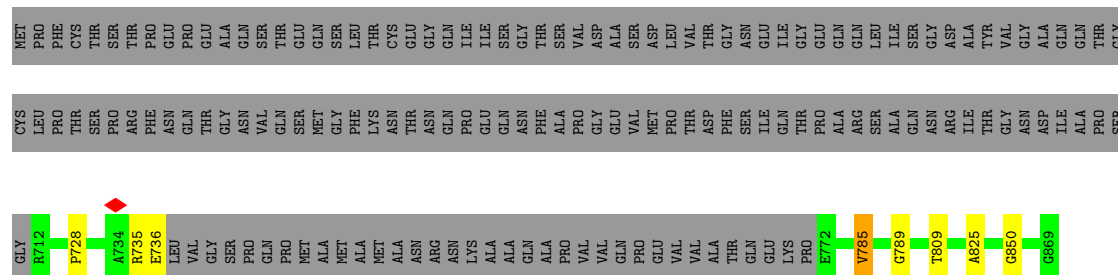
- Molecule 2: Carboxysome shell vertex protein CsoS4A



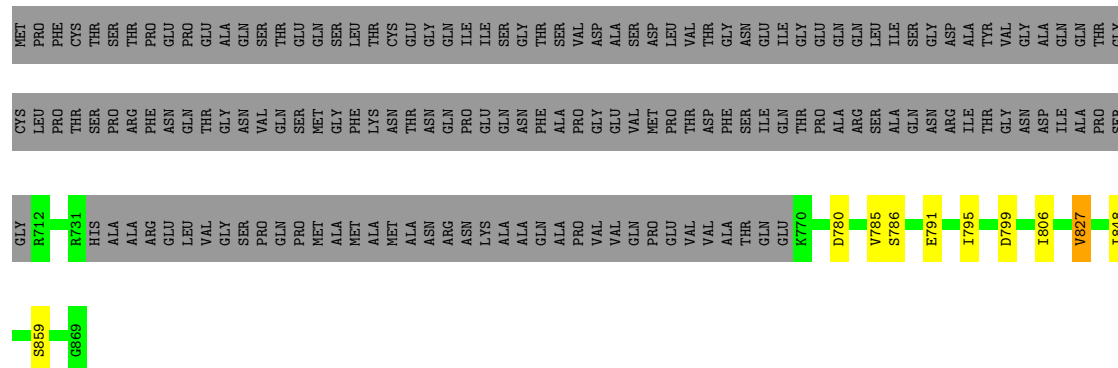
- Chain z: 89% 8% .

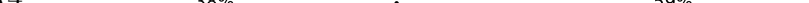


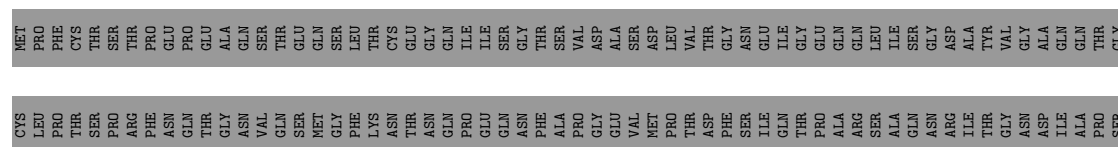
- Chain A2:  41% 0% 56%



- Chain A3:  39% . 57%

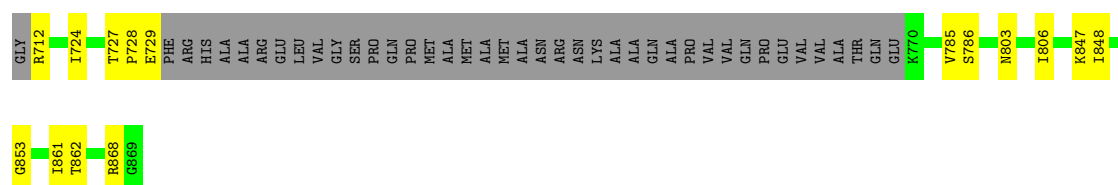
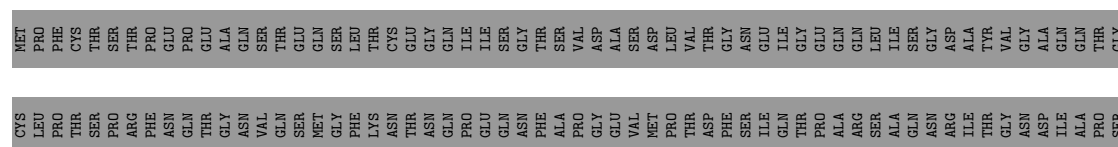


- Chain A4:  38% . 59%

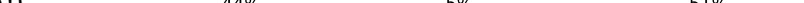


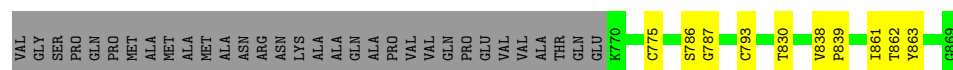
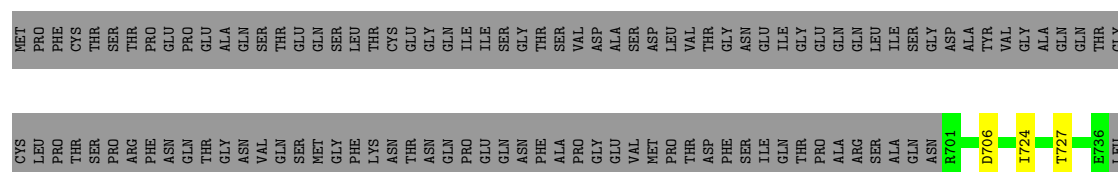
- Molecule 3: Carboxysome assembly protein CsoS2B

Chain A5: 

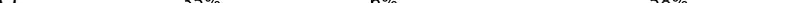


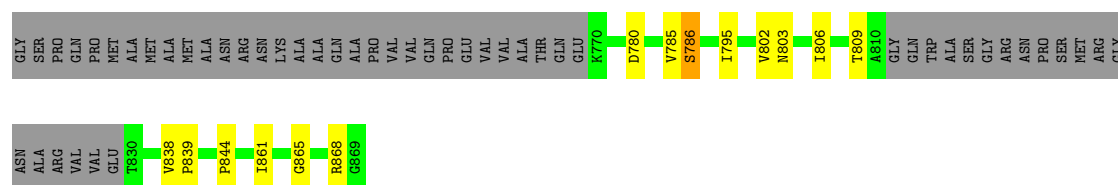
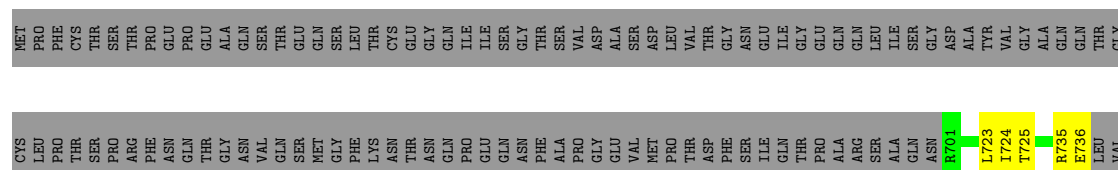
- Molecule 3: Carboxysome assembly protein CsoS2B

Chain A6:  44% 5% 51%



- Molecule 3: Carboxysome assembly protein CsoS2B

Chain A7:  35% 6% 58%



- Molecule 3: Carboxysome assembly protein CsoS2B

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

ASP	TRP	ASP	GLY	PHE	MET
LEU	ILE	TRP	SER	ALA	PRO
THR	VAL	ASN	PRO	GLY	CYS
TYR	ASN	GLN	GLN	GLU	THR
SER	LYS	MET	MET	VAL	SER
HIS	ILE	ALA	ALA	MET	THR
GLY	THR	MET	MET	PRO	PRO
ALA	THR	ALA	ALA	THR	GLU
ARG	GLY	MET	ASP	ASP	PRO
GLY	THR	ALA	PHE	PHE	GLU
ALA	THR	ASN	ASN	SER	ALA
GLY	GLN	ARG	ARG	ILE	GLN
GLN	GLN	ASN	ASN	GLN	GLN
ALA	ALA	LYS	THR	PRO	S604
ALA	ALA	ALA	ALA	PRO	T605
SER	SER	ALA	ALA	ALA	E606
GLY	GLY	GLN	GLN	ARG	Q607
ASN	ASN	ALA	SER	SER	S608
PRO	PRO	VAL	VAL	ALA	L609
SER	SER	VAL	ASN	GLN	T610
MET	MET	GLN	GLN	ASN	Q623
ARG	ARG	PRO	ILE	ILE	L626
GLY	GLY	GLU	THR	THR	V627
ASN	ASN	VAL	GLY	GLY	T628
ALA	ALA	VAL	ASN	ASN	G629
ARG	ARG	ALA	ASP	ASP	Q636
VAL	VAL	THR	THR	ILE	Q647
VAL	VAL	GLN	GLN	ALA	C651
GLU	GLU	GLU	PRO	PRO	LEU
THR	THR	LYS	SER	SER	PRO
ALA	ALA	GLU	GLY	GLY	THR
PHE	PHE	LEU	ILE	ILE	THR
ALA	ALA	CYS	VAL	GLY	SER
ASN	ASN	ALA	ALA	PRO	PRO
ARG	ARG	ALA	GLY	GLY	ARG
ASN	ASN	VAL	ARG	MET	PHE
PRO	PRO	SER	SER	LEU	ASN
LYS	LYS	ASP	ASP	ALA	GLN
PRO	PRO	GLN	GLN	THR	GLN
GLU	GLU	MET	GLY	GLY	THR
LYS	LYS	ASP	LEU	VAL	ASN
PRO	PRO	ARG	ILE	THR	GLN
GLY	GLY	VAL	THR	THR	SER
SER	SER	SER	GLY	GLY	MET
LYS	LYS	LYS	GLY	THR	GLY
ILE	ILE	THR	GLU	PRO	PHE
THR	THR	GLY	GLY	GLU	LYS
GLY	GLY	LYS	LYS	PHE	ASN
SER	SER	SER	ARG	ARG	LYS
GLY	GLY	CYS	THR	HIS	THR
ASN	ASN	GLY	ALA	ALA	ASN
ASP	ASP	ILE	ARG	ALA	GLN
THR	THR	THR	ILE	ARG	GLN
GLN	GLN	GLY	THR	GLU	GLU
GLY	GLY	ASP	GLY	LEU	GLN
				VAL	ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3655	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.598	Depositor
Minimum map value	-0.684	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	423.87695, 428.9231, 483.16925	wwPDB
Map dimensions	336, 340, 383	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2615385, 1.2615385, 1.2615385	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	0	0.34	0/662	0.60	2/897 (0.2%)
1	2	0.33	0/662	0.52	0/897
1	3	0.54	0/662	0.87	0/897
1	5	0.45	0/662	0.64	0/897
1	6	0.34	0/662	0.53	0/897
1	7	0.40	0/662	0.57	0/897
1	8	0.47	1/662 (0.2%)	0.71	0/897
1	9	0.25	0/662	0.39	0/897
1	A	0.29	0/662	0.52	1/897 (0.1%)
1	A1	0.28	0/662	0.50	1/897 (0.1%)
1	B	0.55	0/662	0.84	0/897
1	C	0.52	0/662	0.79	1/897 (0.1%)
1	D	0.23	0/662	0.41	0/897
1	E	0.41	0/662	0.72	2/897 (0.2%)
1	F	0.26	0/662	0.49	1/897 (0.1%)
1	G	0.56	1/662 (0.2%)	0.78	1/897 (0.1%)
1	H	0.16	0/662	0.26	0/897
1	I	0.45	0/662	0.72	1/897 (0.1%)
1	J	0.59	1/662 (0.2%)	0.80	3/897 (0.3%)
1	K	0.54	0/662	0.78	2/897 (0.2%)
1	L	0.53	0/662	0.80	0/897
1	M	0.62	0/662	0.98	1/897 (0.1%)
1	N	0.53	0/662	0.81	0/897
1	O	0.54	0/662	0.82	0/897
1	P	0.45	0/662	0.71	0/897
1	Q	0.51	0/662	0.75	1/897 (0.1%)
1	R	0.43	0/662	0.74	1/897 (0.1%)
1	S	0.30	0/662	0.53	1/897 (0.1%)
1	T	0.27	0/662	0.53	0/897
1	U	0.65	0/662	1.03	2/897 (0.2%)
1	V	0.43	0/662	0.65	0/897
1	W	0.56	0/662	0.85	1/897 (0.1%)
1	X	0.55	1/662 (0.2%)	0.80	2/897 (0.2%)
1	Y	0.69	0/662	0.97	2/897 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	0.38	0/662	0.56	0/897
1	a	0.46	0/662	0.74	1/897 (0.1%)
1	b	0.32	0/662	0.52	0/897
1	c	0.55	0/662	0.84	0/897
1	d	0.16	0/662	0.29	0/897
1	e	0.59	0/662	0.84	0/897
1	f	0.31	0/662	0.57	0/897
1	g	0.29	0/662	0.51	0/897
1	h	0.16	0/662	0.29	0/897
1	i	0.22	0/662	0.44	0/897
1	j	0.41	0/662	0.66	0/897
1	k	0.47	2/662 (0.3%)	0.77	2/897 (0.2%)
1	l	0.41	0/662	0.66	1/897 (0.1%)
1	m	0.49	0/662	0.74	1/897 (0.1%)
1	n	0.49	0/662	0.63	2/897 (0.2%)
1	o	0.25	0/662	0.46	1/897 (0.1%)
1	p	0.32	0/662	0.46	0/897
1	q	0.37	0/662	0.67	0/897
1	r	0.43	0/662	0.68	0/897
1	s	0.40	0/662	0.66	1/897 (0.1%)
1	t	0.34	0/662	0.58	1/897 (0.1%)
1	u	0.35	0/662	0.58	0/897
1	v	0.34	0/662	0.61	1/897 (0.1%)
2	l	0.36	0/620	0.58	0/843
2	4	0.50	0/620	0.75	0/843
2	w	0.69	0/620	0.81	0/843
2	x	0.24	0/620	0.34	0/843
2	y	0.52	0/620	0.74	0/843
2	z	0.38	0/620	0.59	0/843
3	A2	0.67	0/923	1.08	2/1243 (0.2%)
3	A3	0.58	0/899	0.94	1/1211 (0.1%)
3	A4	0.73	0/855	1.24	4/1153 (0.3%)
3	A5	0.58	0/876	0.95	2/1181 (0.2%)
3	A6	0.58	0/1017	0.99	3/1371 (0.2%)
3	A7	0.64	0/869	1.13	1/1170 (0.1%)
3	X1	0.67	0/337	1.15	2/456 (0.4%)
3	X2	0.48	0/337	0.90	1/456 (0.2%)
All	All	0.46	6/47567 (0.0%)	0.73	53/64428 (0.1%)

All (6) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	60	ALA	C-O	-6.29	1.16	1.24
1	G	28	THR	C-O	-6.03	1.17	1.24
1	J	83	ARG	C-O	-5.51	1.17	1.24
1	8	23	ALA	C-O	-5.43	1.17	1.24
1	k	28	THR	C-O	-5.36	1.17	1.24
1	k	26	ALA	C-O	-5.03	1.18	1.24

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	73	ASP	CB-CA-C	7.73	123.62	110.79
3	A7	786	SER	N-CA-C	7.67	119.72	111.36
1	F	73	ASP	CB-CA-C	7.34	124.22	110.63
1	Q	16	GLY	CA-C-O	-7.24	117.24	122.45
1	U	16	GLY	CA-C-O	-7.14	117.16	122.37
3	A3	786	SER	N-CA-C	6.47	118.12	111.14
3	A2	728	PRO	N-CA-C	6.42	122.66	113.47
1	E	42	GLY	CA-C-O	-6.40	116.89	121.88
3	A4	863	TYR	CA-C-O	-6.37	114.19	121.58
3	A5	786	SER	N-CA-C	6.33	118.26	111.36
3	A6	786	SER	N-CA-C	6.25	118.18	111.36
1	k	74	GLY	N-CA-C	6.10	118.67	110.43
3	X2	606	GLU	N-CA-C	-6.03	105.78	113.02
1	I	74	GLY	N-CA-C	5.96	118.47	110.43
1	m	73	ASP	CB-CA-C	5.92	120.92	110.85
1	Y	53	GLU	CA-C-O	-5.76	115.54	121.87
1	a	73	ASP	CB-CA-C	5.69	120.24	110.79
1	W	53	GLU	CA-C-O	-5.65	115.31	121.87
3	A6	787	GLY	CA-C-O	-5.65	116.00	120.91
3	A4	787	GLY	CA-C-O	-5.60	115.25	120.57
1	o	73	ASP	CB-CA-C	5.57	120.93	110.63
1	t	73	ASP	CB-CA-C	5.56	120.02	110.79
1	J	74	GLY	N-CA-C	5.54	118.39	110.46
1	X	60	ALA	CA-C-O	-5.54	115.18	121.00
3	A5	861	ILE	N-CA-C	-5.49	100.67	108.58
3	X1	606	GLU	N-CA-C	-5.49	99.97	108.31
1	0	53	GLU	CA-C-O	-5.44	115.68	121.94
1	s	73	ASP	CB-CA-C	5.43	119.80	110.79
1	U	95	ALA	CA-C-O	-5.41	115.09	120.66
1	G	42	GLY	CA-C-O	-5.38	117.68	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	73	ASP	CB-CA-C	5.35	119.64	110.01
3	A4	786	SER	N-CA-C	5.32	116.89	111.14
1	n	83	ARG	CA-C-O	-5.31	114.56	120.66
1	A1	73	ASP	N-CA-C	-5.30	105.50	111.28
3	A6	727	THR	CB-CA-C	5.28	119.28	109.51
1	l	13	GLU	CA-C-O	-5.27	115.06	121.28
1	k	26	ALA	CA-C-O	-5.26	114.97	120.55
1	M	53	GLU	CA-C-O	-5.26	115.77	121.87
1	n	42	GLY	CA-C-O	-5.25	117.67	122.24
1	A	45	TYR	CA-C-O	-5.22	115.27	120.96
1	E	74	GLY	CA-C-O	-5.21	117.09	122.25
1	X	58	ASN	N-CA-C	-5.21	105.50	111.07
1	0	73	ASP	CB-CA-C	5.21	119.44	110.79
3	A2	850	GLY	CA-C-O	-5.18	115.50	121.46
1	K	61	VAL	N-CA-C	-5.12	105.40	110.62
1	J	83	ARG	CA-C-O	-5.09	114.67	120.32
1	C	65	ALA	N-CA-C	-5.08	105.63	111.07
3	A4	784	ARG	N-CA-C	-5.07	105.44	110.97
1	K	69	GLU	CA-C-O	-5.05	115.17	120.63
1	v	73	ASP	CB-CA-C	5.03	119.40	110.85
1	R	78	ALA	CA-C-O	-5.02	114.93	120.30
3	X1	607	GLN	N-CA-C	-5.01	101.67	109.24
1	S	73	ASP	CB-CA-C	5.01	119.90	110.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	656	0	677	3	0
1	2	656	0	677	4	0
1	3	656	0	677	1	0
1	5	656	0	677	6	0
1	6	656	0	677	9	0
1	7	656	0	677	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	656	0	677	3	0
1	9	656	0	677	5	0
1	A	656	0	677	7	0
1	A1	656	0	677	6	0
1	B	656	0	677	3	0
1	C	656	0	677	5	0
1	D	656	0	677	4	0
1	E	656	0	677	2	0
1	F	656	0	677	0	0
1	G	656	0	677	8	0
1	H	656	0	677	6	0
1	I	656	0	677	4	0
1	J	656	0	677	4	0
1	K	656	0	677	3	0
1	L	656	0	677	3	0
1	M	656	0	677	4	0
1	N	656	0	677	6	0
1	O	656	0	677	5	0
1	P	656	0	677	4	0
1	Q	656	0	677	2	0
1	R	656	0	677	4	0
1	S	656	0	677	2	0
1	T	656	0	677	5	0
1	U	656	0	677	8	0
1	V	656	0	677	7	0
1	W	656	0	677	10	0
1	X	656	0	677	4	0
1	Y	656	0	677	9	0
1	Z	656	0	677	5	0
1	a	656	0	677	6	0
1	b	656	0	677	10	0
1	c	656	0	677	5	0
1	d	656	0	677	7	0
1	e	656	0	677	6	0
1	f	656	0	677	2	0
1	g	656	0	677	9	0
1	h	656	0	677	11	0
1	i	656	0	677	7	0
1	j	656	0	677	3	0
1	k	656	0	677	10	0
1	l	656	0	677	8	0
1	m	656	0	677	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n	656	0	677	6	0
1	o	656	0	677	8	0
1	p	656	0	677	4	0
1	q	656	0	677	8	0
1	r	656	0	677	6	0
1	s	656	0	677	5	0
1	t	656	0	677	6	0
1	u	656	0	677	6	0
1	v	656	0	677	6	0
2	1	608	0	625	5	0
2	4	608	0	625	4	0
2	w	608	0	625	14	0
2	x	608	0	625	9	0
2	y	608	0	625	7	0
2	z	608	0	625	9	0
3	A2	908	0	880	5	0
3	A3	884	0	864	10	0
3	A4	842	0	819	1	0
3	A5	862	0	842	13	0
3	A6	1000	0	975	6	0
3	A7	856	0	836	20	0
3	X1	337	0	311	3	0
3	X2	337	0	311	5	0
All	All	47066	0	48177	306	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 3.

All (306) 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:g:7:ILE:O	1:g:51:ARG:NH1	2.23	0.71
1:q:77:ALA:HB2	1:t:72:GLY:HA2	1.72	0.71
1:r:77:ALA:HB2	1:v:72:GLY:HA2	1.73	0.69
1:g:79:HIS:NE2	1:i:22:GLU:OE1	2.21	0.68
1:i:51:ARG:NH2	1:i:89:GLU:OE2	2.27	0.68
1:k:36:VAL:HG21	1:k:51:ARG:HG2	1.76	0.67
2:x:29:GLU:OE2	2:x:29:GLU:N	2.26	0.67
1:i:32:GLU:HB2	1:p:7:ILE:HD11	1.77	0.67
1:G:77:ALA:HB2	1:J:72:GLY:HA2	1.77	0.66
1:h:15:ARG:NH1	1:h:73:ASP:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:1:MET:CE	2:z:51:LEU:HD21	2.27	0.65
1:G:80:ILE:HD11	3:A5:848:ILE:HD11	1.80	0.64
2:z:1:MET:HE1	2:z:51:LEU:HD21	1.78	0.64
1:q:72:GLY:HA2	1:v:77:ALA:HB2	1.79	0.64
2:w:23:PRO:HG2	2:w:40:ASP:HB3	1.79	0.64
2:w:18:ASP:C	2:w:20:GLY:N	2.55	0.63
1:e:45:TYR:OH	1:h:73:ASP:OD2	2.16	0.63
1:n:61:VAL:HG12	3:A3:848:ILE:HD11	1.80	0.63
1:g:22:GLU:OE1	1:h:79:HIS:NE2	2.27	0.62
1:p:38:ARG:O	1:p:38:ARG:NH1	2.34	0.61
1:s:72:GLY:HA2	1:t:77:ALA:HB2	1.81	0.61
1:b:12:ILE:HD12	1:b:27:MET:SD	2.41	0.61
1:l:61:VAL:HG12	3:A7:724:ILE:CD1	2.31	0.59
1:k:12:ILE:HD12	1:k:27:MET:SD	2.42	0.59
2:1:77:ILE:HD13	2:w:10:LEU:HD11	1.84	0.59
2:1:10:LEU:HD11	2:z:77:ILE:HD12	1.85	0.59
1:m:77:ALA:HB2	1:o:72:GLY:HA2	1.85	0.59
1:7:80:ILE:HD11	3:A6:724:ILE:HD11	1.85	0.59
1:I:88:VAL:HG21	1:K:25:ASP:HA	1.84	0.59
1:5:88:VAL:HG21	1:7:25:ASP:HA	1.85	0.59
1:O:12:ILE:HD12	1:O:27:MET:SD	2.43	0.58
1:a:77:ALA:HB2	1:c:72:GLY:HA2	1.85	0.58
1:N:12:ILE:HD12	1:N:27:MET:HE3	1.85	0.58
3:A5:803:ASN:OD1	3:A5:806:ILE:HD12	2.04	0.58
2:x:1:MET:HE1	2:y:39:VAL:HG23	1.86	0.57
1:U:12:ILE:HD12	1:U:27:MET:HE2	1.87	0.57
1:7:12:ILE:HD12	1:7:27:MET:SD	2.43	0.57
1:b:38:ARG:O	1:b:38:ARG:NH1	2.37	0.57
1:G:9:LEU:HD11	1:G:49:LEU:HD12	1.87	0.56
2:1:42:ILE:O	2:1:42:ILE:HD12	2.06	0.56
1:V:12:ILE:HD12	1:V:27:MET:SD	2.46	0.55
1:o:19:PRO:HG3	1:o:72:GLY:HA3	1.88	0.55
1:W:31:ALA:HB3	1:W:60:ALA:HB2	1.89	0.55
2:x:1:MET:N	2:y:70:ASP:OD1	2.39	0.55
1:B:12:ILE:HD12	1:B:27:MET:SD	2.47	0.55
2:w:18:ASP:O	2:w:19:MET:C	2.48	0.55
1:o:38:ARG:O	1:o:38:ARG:NH1	2.39	0.55
1:2:12:ILE:HD12	1:2:27:MET:SD	2.46	0.54
1:l:69:GLU:OE1	3:A7:723:LEU:HD13	2.07	0.54
1:l:79:HIS:ND1	3:A7:725:THR:OG1	2.37	0.54
2:w:2:LYS:HE3	2:w:29:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:77:ILE:HG21	2:z:80:TRP:HB2	1.88	0.54
1:H:49:LEU:HD11	1:H:93:PRO:HD2	1.88	0.54
1:R:61:VAL:HB	1:R:80:ILE:HD11	1.90	0.54
1:r:49:LEU:HD11	1:r:93:PRO:HD2	1.89	0.54
1:f:75:LEU:HD23	3:X2:626:LEU:HD12	1.90	0.53
1:9:89:GLU:O	1:9:94:LYS:NZ	2.41	0.53
3:A7:838:VAL:HG22	3:A7:839:PRO:HD2	1.90	0.53
1:k:80:ILE:CD1	3:A7:785:VAL:HG11	2.39	0.52
3:A7:802:VAL:HG21	3:A7:809:THR:HG21	1.90	0.52
1:R:80:ILE:HD12	3:A3:806:ILE:HG21	1.92	0.52
1:Y:80:ILE:CD1	3:A5:785:VAL:HG11	2.39	0.52
3:A2:735:ARG:O	3:A2:736:GLU:C	2.52	0.52
1:W:81:ILE:HG22	1:W:83:ARG:O	2.09	0.52
2:y:80:TRP:O	2:y:81:ASN:C	2.53	0.52
2:w:18:ASP:O	2:w:20:GLY:N	2.43	0.51
1:B:24:ALA:HB2	1:B:48:VAL:HG21	1.92	0.51
1:Y:17:LEU:N	1:d:13:GLU:OE2	2.40	0.51
1:h:12:ILE:HD12	1:h:27:MET:SD	2.50	0.51
1:S:70:ARG:NH2	1:n:66:ASP:OD2	2.43	0.51
1:8:12:ILE:HD12	1:8:27:MET:SD	2.50	0.51
1:l:25:ASP:HA	1:o:88:VAL:HG21	1.93	0.51
1:J:24:ALA:HB1	1:J:35:LEU:CD1	2.40	0.51
1:K:45:TYR:CE1	1:K:76:VAL:HG21	2.46	0.51
1:d:35:LEU:HD11	1:d:48:VAL:HG13	1.93	0.50
1:Z:77:ALA:HB2	1:d:72:GLY:HA2	1.93	0.50
1:d:12:ILE:HD12	1:d:27:MET:SD	2.51	0.50
1:A1:94:LYS:HA	1:A1:94:LYS:HE2	1.94	0.50
2:y:42:ILE:HG22	2:y:43:GLY:H	1.77	0.50
1:r:72:GLY:HA2	1:u:77:ALA:HB2	1.94	0.50
3:A3:795:ILE:N	3:A3:795:ILE:HD12	2.27	0.50
1:C:11:MET:HE3	1:C:79:HIS:HB3	1.94	0.50
1:U:15:ARG:HD2	3:A3:827:VAL:HG12	1.93	0.50
3:A6:830:THR:HG23	3:A6:830:THR:O	2.12	0.50
1:k:36:VAL:HG21	1:k:51:ARG:CG	2.41	0.50
1:E:22:GLU:HG2	1:E:71:VAL:HG21	1.92	0.49
1:G:18:VAL:HG22	1:L:11:MET:HB3	1.94	0.49
1:a:62:ARG:NH2	3:A5:853:GLY:O	2.45	0.49
1:0:62:ARG:NH1	3:X2:636:GLN:O	2.46	0.49
1:5:72:GLY:HA2	1:6:77:ALA:HB2	1.94	0.49
1:W:36:VAL:HG11	1:W:51:ARG:CG	2.43	0.49
1:g:12:ILE:HD12	1:g:27:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:11:MET:HG2	1:v:49:LEU:HD23	1.93	0.49
1:W:22:GLU:OE1	1:W:67:ALA:HB1	2.13	0.49
1:C:68:CYS:SG	1:C:75:LEU:HD13	2.52	0.49
1:P:28:THR:O	1:c:83:ARG:NH1	2.43	0.48
1:A:49:LEU:HD23	1:A:49:LEU:H	1.78	0.48
1:s:66:ASP:OD1	3:X2:610:THR:HG21	2.13	0.48
1:K:68:CYS:SG	1:K:75:LEU:HD13	2.54	0.48
3:A5:728:PRO:O	3:A5:729:GLU:C	2.56	0.48
1:C:12:ILE:HD12	1:C:27:MET:SD	2.54	0.48
1:X:68:CYS:SG	1:X:75:LEU:HD13	2.53	0.48
1:G:77:ALA:HB2	1:J:72:GLY:CA	2.44	0.47
1:W:36:VAL:HG11	1:W:51:ARG:HG2	1.96	0.47
2:w:18:ASP:HB2	2:w:68:PRO:HG3	1.96	0.47
1:i:7:ILE:HG22	1:i:7:ILE:O	2.13	0.47
1:q:77:ALA:HB2	1:t:72:GLY:CA	2.42	0.47
3:A3:780:ASP:OD1	3:A3:780:ASP:C	2.57	0.47
1:V:32:GLU:HG3	1:h:7:ILE:HD11	1.96	0.47
2:x:27:VAL:O	2:x:27:VAL:HG23	2.13	0.47
1:P:27:MET:HE3	1:P:61:VAL:HG22	1.97	0.47
2:z:51:LEU:HD23	2:z:74:ILE:HG12	1.96	0.47
1:0:33:VAL:HB	1:0:50:VAL:HG22	1.96	0.47
1:7:36:VAL:HG11	1:7:51:ARG:HG3	1.96	0.47
2:x:1:MET:N	2:x:1:MET:SD	2.88	0.47
1:a:12:ILE:HD12	1:a:27:MET:SD	2.54	0.47
3:A5:847:LYS:HD2	3:A5:847:LYS:O	2.14	0.47
1:J:22:GLU:HG2	1:J:71:VAL:HG21	1.97	0.47
1:R:80:ILE:HD12	3:A3:806:ILE:CG2	2.45	0.47
1:u:11:MET:HG2	1:u:49:LEU:HD12	1.97	0.47
1:D:36:VAL:HG11	1:D:51:ARG:CG	2.45	0.46
1:V:32:GLU:CG	1:h:7:ILE:HD11	2.45	0.46
1:r:72:GLY:CA	1:u:77:ALA:HB2	2.45	0.46
1:M:24:ALA:HB2	1:M:48:VAL:HG21	1.96	0.46
1:g:22:GLU:CD	1:h:79:HIS:HE2	2.18	0.46
1:s:72:GLY:CA	1:t:77:ALA:HB2	2.46	0.46
1:M:82:ALA:HB3	1:Z:30:ALA:O	2.16	0.46
1:e:7:ILE:O	1:e:51:ARG:NH2	2.44	0.46
1:2:88:VAL:HG21	1:6:25:ASP:HA	1.97	0.46
1:T:77:ALA:HB2	1:X:72:GLY:CA	2.46	0.46
1:D:15:ARG:HH11	3:A2:825:ALA:HB3	1.80	0.46
1:X:83:ARG:NH1	1:n:29:LYS:O	2.48	0.46
1:9:77:ALA:HB2	1:A1:72:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:78:ALA:HB1	3:A7:724:ILE:HD13	1.96	0.46
1:a:22:GLU:HG2	1:a:71:VAL:HG21	1.98	0.46
2:y:9:THR:HA	2:y:25:LEU:HD13	1.97	0.46
1:C:23:ALA:O	1:C:27:MET:HG3	2.16	0.45
1:D:36:VAL:HG11	1:D:51:ARG:HG3	1.97	0.45
1:O:13:GLU:HG3	1:Q:18:VAL:HG23	1.99	0.45
1:o:9:LEU:HD23	1:o:11:MET:HE2	1.98	0.45
2:x:42:ILE:HD13	2:x:75:GLY:N	2.31	0.45
1:A:32:GLU:O	1:A:32:GLU:OE1	2.35	0.45
1:B:35:LEU:HA	1:B:50:VAL:HG12	1.99	0.45
1:T:12:ILE:HD12	1:T:27:MET:SD	2.56	0.45
1:Y:12:ILE:HD12	1:Y:27:MET:SD	2.56	0.45
2:w:74:ILE:HD12	2:x:19:MET:SD	2.57	0.45
1:s:77:ALA:HB1	1:u:18:VAL:HG11	1.99	0.45
2:1:70:ASP:OD1	2:z:1:MET:N	2.33	0.45
2:4:1:MET:HG2	2:4:51:LEU:HD21	1.99	0.45
1:b:22:GLU:HG2	1:b:71:VAL:HG21	1.99	0.45
1:5:12:ILE:HG23	1:5:75:LEU:HD11	1.99	0.45
1:V:30:ALA:O	1:h:82:ALA:HB3	2.17	0.45
1:g:80:ILE:HD12	3:A7:806:ILE:HG21	1.99	0.45
1:H:68:CYS:SG	1:H:75:LEU:HD13	2.56	0.45
1:E:68:CYS:SG	1:E:75:LEU:HD13	2.57	0.45
1:k:80:ILE:HD12	3:A7:785:VAL:CG1	2.47	0.45
1:v:41:VAL:HB	1:v:45:TYR:HB2	1.99	0.45
1:i:66:ASP:OD1	3:X1:610:THR:HG21	2.17	0.45
1:5:7:ILE:O	1:5:51:ARG:NH1	2.49	0.45
1:T:18:VAL:HB	1:T:19:PRO:HD3	1.99	0.45
1:l:7:ILE:HD11	1:r:32:GLU:HG3	1.99	0.45
2:w:6:VAL:CG1	2:w:25:LEU:HD13	2.47	0.45
1:T:11:MET:HE3	1:T:79:HIS:HB3	1.99	0.44
1:T:77:ALA:HB2	1:X:72:GLY:HA2	1.98	0.44
1:l:69:GLU:OE1	3:A7:723:LEU:HD22	2.17	0.44
2:w:50:VAL:HB	2:w:73:ILE:HG23	1.98	0.44
1:6:68:CYS:SG	1:6:75:LEU:HD13	2.58	0.44
1:G:18:VAL:HG13	1:L:11:MET:HE3	1.98	0.44
2:w:6:VAL:HG11	2:w:25:LEU:HD13	1.99	0.44
3:A7:803:ASN:N	3:A7:803:ASN:OD1	2.50	0.44
2:w:18:ASP:C	2:w:20:GLY:H	2.26	0.44
3:X2:628:THR:HG22	3:X2:629:GLY:N	2.33	0.44
1:S:29:LYS:O	1:k:83:ARG:NH1	2.50	0.44
1:e:18:VAL:HG22	1:j:11:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:62:ARG:NH1	3:X2:623:ALA:O	2.51	0.44
1:H:58:ASN:O	1:H:62:ARG:HG2	2.16	0.44
2:4:51:LEU:HD23	2:4:52:CYS:N	2.32	0.44
1:b:11:MET:HG2	1:b:49:LEU:HD22	1.99	0.44
1:h:11:MET:HE3	1:h:11:MET:HB2	1.96	0.44
2:4:51:LEU:HD23	2:4:51:LEU:C	2.43	0.44
1:5:72:GLY:CA	1:6:77:ALA:HB2	2.48	0.44
1:a:69:GLU:OE2	1:a:75:LEU:HB3	2.17	0.44
1:e:17:LEU:N	1:j:13:GLU:OE2	2.41	0.44
1:h:7:ILE:HD12	1:h:7:ILE:C	2.43	0.44
1:9:13:GLU:OE2	1:A1:17:LEU:N	2.49	0.43
1:I:61:VAL:HG21	1:I:80:ILE:HD13	2.00	0.43
1:n:12:ILE:HD12	1:n:27:MET:CE	2.48	0.43
1:3:77:ALA:HB2	1:8:72:GLY:HA2	2.00	0.43
3:A2:809:THR:O	3:A2:809:THR:CG2	2.66	0.43
3:A7:795:ILE:HD13	3:A7:795:ILE:N	2.34	0.43
1:U:77:ALA:HB2	1:W:72:GLY:HA2	1.99	0.43
1:W:32:GLU:HG3	1:W:32:GLU:O	2.19	0.43
1:Y:77:ALA:HB2	1:b:72:GLY:CA	2.48	0.43
1:j:62:ARG:NH2	3:A6:706:ASP:OD2	2.52	0.43
1:d:68:CYS:SG	1:d:75:LEU:HD13	2.59	0.43
3:X1:607:GLN:HA	3:X1:607:GLN:NE2	2.34	0.43
1:Y:80:ILE:HD12	3:A5:785:VAL:HG11	2.00	0.43
3:A7:735:ARG:O	3:A7:736:GLU:C	2.62	0.43
1:8:35:LEU:HA	1:8:50:VAL:HG12	2.01	0.43
1:A:35:LEU:HA	1:A:50:VAL:HG12	2.00	0.43
1:U:36:VAL:HG11	1:U:51:ARG:HG3	1.99	0.43
2:x:1:MET:HE1	2:y:39:VAL:CG2	2.48	0.43
1:b:9:LEU:HD13	1:b:51:ARG:HD3	2.00	0.43
1:q:11:MET:HE3	1:q:79:HIS:HB3	1.99	0.43
1:t:31:ALA:HB3	1:t:60:ALA:HB2	2.01	0.43
1:2:13:GLU:OE2	1:6:17:LEU:N	2.52	0.43
1:A:7:ILE:O	1:A:7:ILE:HG22	2.17	0.43
1:e:80:ILE:CD1	3:A5:806:ILE:HG21	2.49	0.43
2:4:51:LEU:HD22	2:4:74:ILE:CG1	2.49	0.42
1:O:25:ASP:HA	1:P:88:VAL:HG21	2.01	0.42
1:V:11:MET:HG2	1:V:49:LEU:HD23	2.01	0.42
1:Y:11:MET:HB3	1:b:18:VAL:HG22	2.00	0.42
1:G:80:ILE:HD11	3:A5:848:ILE:CD1	2.47	0.42
1:N:36:VAL:HG22	1:N:49:LEU:O	2.19	0.42
1:O:72:GLY:CA	1:P:77:ALA:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:78:ALA:HB3	3:A7:861:ILE:HD13	2.01	0.42
2:z:42:ILE:O	2:z:42:ILE:HG23	2.19	0.42
3:A7:844:PRO:HB2	3:A7:868:ARG:H	1.84	0.42
1:5:22:GLU:OE1	1:6:79:HIS:NE2	2.51	0.42
1:H:9:LEU:HD11	1:H:49:LEU:HD12	2.01	0.42
1:N:88:VAL:HG21	1:R:25:ASP:HA	2.01	0.42
1:k:45:TYR:OH	1:n:73:ASP:OD2	2.21	0.42
3:A2:809:THR:O	3:A2:809:THR:HG22	2.18	0.42
1:A1:11:MET:HE3	1:A1:79:HIS:HB3	2.01	0.42
1:Z:77:ALA:HB2	1:d:72:GLY:CA	2.49	0.42
1:c:36:VAL:HG22	1:c:49:LEU:O	2.20	0.42
1:t:32:GLU:O	1:t:32:GLU:HG2	2.19	0.42
3:A7:802:VAL:HG11	3:A7:809:THR:HG21	2.02	0.42
1:A:41:VAL:O	1:A:41:VAL:HG12	2.20	0.42
1:g:7:ILE:CD1	1:k:32:GLU:HB2	2.49	0.42
1:0:35:LEU:HA	1:0:50:VAL:HG23	2.01	0.42
1:W:80:ILE:HD12	3:A3:785:VAL:HG13	2.00	0.42
1:k:41:VAL:HB	1:k:45:TYR:HB2	2.00	0.42
1:r:77:ALA:HB2	1:v:72:GLY:CA	2.44	0.42
1:u:59:ALA:HB1	3:X1:619:THR:HG23	2.01	0.42
3:A3:799:ASP:OD1	3:A3:799:ASP:C	2.62	0.42
1:U:68:CYS:SG	1:U:75:LEU:HD13	2.59	0.42
1:Z:25:ASP:HA	1:c:88:VAL:HG21	2.02	0.42
1:m:65:ALA:CB	3:A7:861:ILE:HD11	2.50	0.42
1:9:35:LEU:HA	1:9:50:VAL:HG12	2.01	0.42
1:I:12:ILE:HD12	1:I:27:MET:SD	2.59	0.42
1:N:72:GLY:HA2	1:Q:77:ALA:HB2	2.01	0.42
1:a:77:ALA:HB2	1:c:72:GLY:CA	2.48	0.42
2:w:15:ARG:NH2	2:w:20:GLY:O	2.52	0.42
1:7:35:LEU:HD11	1:7:48:VAL:CG2	2.49	0.42
1:C:57:VAL:HG11	1:C:80:ILE:HG23	2.02	0.42
1:Y:13:GLU:OE2	1:b:17:LEU:N	2.53	0.42
1:o:70:ARG:NH2	3:A7:865:GLY:O	2.53	0.42
1:M:9:LEU:HD23	1:M:11:MET:HE2	2.01	0.41
1:Z:61:VAL:HG12	3:A5:724:ILE:CD1	2.50	0.41
1:o:36:VAL:HG11	1:o:51:ARG:CG	2.50	0.41
2:w:19:MET:O	2:w:67:TYR:OH	2.33	0.41
1:M:66:ASP:OD1	3:A5:712:ARG:NH1	2.52	0.41
1:9:77:ALA:HB2	1:A1:72:GLY:CA	2.50	0.41
1:H:9:LEU:HD13	1:H:51:ARG:HD3	2.03	0.41
1:I:54:THR:O	1:I:58:ASN:ND2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:80:ILE:CD1	3:A3:785:VAL:CG1	2.98	0.41
1:e:36:VAL:HG22	1:e:49:LEU:O	2.21	0.41
1:s:77:ALA:HB2	1:u:72:GLY:CA	2.49	0.41
2:1:24:LEU:O	2:1:25:LEU:HD12	2.21	0.41
1:7:35:LEU:HD12	1:7:50:VAL:HG12	2.02	0.41
1:N:81:ILE:HG22	1:N:83:ARG:O	2.21	0.41
2:x:42:ILE:HD11	2:y:16:ILE:HG23	2.02	0.41
1:U:72:GLY:HA2	1:V:77:ALA:HB2	2.02	0.41
1:g:36:VAL:HG22	1:g:49:LEU:O	2.20	0.41
1:l:88:VAL:HG21	1:p:25:ASP:HA	2.01	0.41
1:7:9:LEU:HD13	1:7:51:ARG:HD3	2.03	0.41
1:A:27:MET:HG3	1:A:64:GLY:HA3	2.03	0.41
3:A6:775:CYS:HA	3:A6:793:CYS:HA	2.03	0.41
1:b:27:MET:HE2	1:b:50:VAL:HG11	2.03	0.41
1:2:11:MET:HG3	1:6:18:VAL:HG22	2.03	0.41
1:W:23:ALA:O	1:W:27:MET:HG3	2.20	0.41
1:k:80:ILE:CD1	3:A7:785:VAL:CG1	2.99	0.41
1:6:65:ALA:CB	3:A6:861:ILE:HD11	2.50	0.41
1:G:32:GLU:C	1:G:32:GLU:OE2	2.64	0.41
1:L:80:ILE:HG13	3:A4:785:VAL:CG1	2.50	0.41
1:d:7:ILE:O	1:d:8:ALA:C	2.64	0.41
1:i:10:GLY:O	1:i:50:VAL:HG22	2.20	0.41
1:i:36:VAL:HG23	1:i:49:LEU:HB2	2.03	0.41
1:m:65:ALA:HB3	3:A7:861:ILE:HD11	2.01	0.41
1:q:11:MET:HB3	1:q:49:LEU:HD22	2.02	0.41
1:q:49:LEU:HD12	1:q:93:PRO:HD2	2.02	0.41
2:z:42:ILE:O	2:z:42:ILE:CG2	2.69	0.41
3:A6:838:VAL:HG12	3:A6:839:PRO:HD2	2.03	0.41
1:A:49:LEU:HD23	1:A:49:LEU:N	2.34	0.41
1:U:84:VAL:HG12	1:U:88:VAL:HB	2.02	0.41
1:q:48:VAL:HG23	1:q:48:VAL:O	2.21	0.41
3:A2:785:VAL:HG11	3:A2:789:GLY:HA3	2.03	0.41
3:A5:806:ILE:HD12	3:A5:806:ILE:H	1.85	0.41
1:N:12:ILE:HD12	1:N:27:MET:CE	2.49	0.40
1:h:88:VAL:O	1:h:88:VAL:HG12	2.21	0.40
1:q:48:VAL:C	1:q:49:LEU:HD23	2.46	0.40
1:H:7:ILE:CD1	1:O:32:GLU:HB2	2.51	0.40
1:U:25:ASP:OD2	1:V:81:ILE:HG21	2.20	0.40
1:n:61:VAL:HG12	3:A3:848:ILE:CD1	2.48	0.40
1:6:36:VAL:HG11	1:6:51:ARG:HG2	2.03	0.40
1:D:9:LEU:HD13	1:D:51:ARG:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:10:GLY:O	1:p:50:VAL:HG22	2.21	0.40
2:z:1:MET:HE3	2:z:51:LEU:HD21	2.01	0.40
1:Y:36:VAL:HG11	1:Y:51:ARG:HG3	2.04	0.40
1:Y:77:ALA:HB2	1:b:72:GLY:HA2	2.03	0.40
1:g:27:MET:HG3	1:g:64:GLY:HA3	2.03	0.40
1:o:7:ILE:O	1:o:7:ILE:HG22	2.22	0.40
3:A5:724:ILE:CG2	3:A5:727:THR:HG23	2.52	0.40
1:v:22:GLU:HA	1:v:22:GLU:OE1	2.20	0.40
1:A1:25:ASP:OD1	1:A1:25:ASP:C	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	2	90/98 (92%)	90 (100%)	0	0	100	100
1	3	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	6	90/98 (92%)	90 (100%)	0	0	100	100
1	7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	8	90/98 (92%)	90 (100%)	0	0	100	100
1	9	90/98 (92%)	90 (100%)	0	0	100	100
1	A	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	A1	90/98 (92%)	90 (100%)	0	0	100	100
1	B	90/98 (92%)	90 (100%)	0	0	100	100
1	C	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D	90/98 (92%)	90 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	90/98 (92%)	90 (100%)	0	0	100	100
1	F	90/98 (92%)	90 (100%)	0	0	100	100
1	G	90/98 (92%)	90 (100%)	0	0	100	100
1	H	90/98 (92%)	90 (100%)	0	0	100	100
1	I	90/98 (92%)	90 (100%)	0	0	100	100
1	J	90/98 (92%)	90 (100%)	0	0	100	100
1	K	90/98 (92%)	90 (100%)	0	0	100	100
1	L	90/98 (92%)	90 (100%)	0	0	100	100
1	M	90/98 (92%)	90 (100%)	0	0	100	100
1	N	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	O	90/98 (92%)	90 (100%)	0	0	100	100
1	P	90/98 (92%)	90 (100%)	0	0	100	100
1	Q	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	R	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	S	90/98 (92%)	90 (100%)	0	0	100	100
1	T	90/98 (92%)	90 (100%)	0	0	100	100
1	U	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	V	90/98 (92%)	90 (100%)	0	0	100	100
1	W	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	X	90/98 (92%)	90 (100%)	0	0	100	100
1	Y	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Z	90/98 (92%)	90 (100%)	0	0	100	100
1	a	90/98 (92%)	90 (100%)	0	0	100	100
1	b	90/98 (92%)	90 (100%)	0	0	100	100
1	c	90/98 (92%)	90 (100%)	0	0	100	100
1	d	90/98 (92%)	90 (100%)	0	0	100	100
1	e	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	f	90/98 (92%)	90 (100%)	0	0	100	100
1	g	90/98 (92%)	90 (100%)	0	0	100	100
1	h	90/98 (92%)	90 (100%)	0	0	100	100
1	i	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	k	90/98 (92%)	90 (100%)	0	0	100	100
1	l	90/98 (92%)	90 (100%)	0	0	100	100
1	m	90/98 (92%)	90 (100%)	0	0	100	100
1	n	90/98 (92%)	90 (100%)	0	0	100	100
1	o	90/98 (92%)	90 (100%)	0	0	100	100
1	p	90/98 (92%)	90 (100%)	0	0	100	100
1	q	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	r	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	s	90/98 (92%)	90 (100%)	0	0	100	100
1	t	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	u	90/98 (92%)	90 (100%)	0	0	100	100
1	v	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
2	1	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
2	4	79/83 (95%)	78 (99%)	0	1 (1%)	9	38
2	w	79/83 (95%)	75 (95%)	3 (4%)	1 (1%)	9	38
2	x	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	y	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	z	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
3	A2	119/279 (43%)	113 (95%)	6 (5%)	0	100	100
3	A3	116/279 (42%)	111 (96%)	5 (4%)	0	100	100
3	A4	111/279 (40%)	106 (96%)	5 (4%)	0	100	100
3	A5	114/279 (41%)	107 (94%)	7 (6%)	0	100	100
3	A6	132/279 (47%)	130 (98%)	2 (2%)	0	100	100
3	A7	111/279 (40%)	105 (95%)	6 (5%)	0	100	100
3	X1	46/279 (16%)	44 (96%)	2 (4%)	0	100	100
3	X2	46/279 (16%)	45 (98%)	1 (2%)	0	100	100
All	All	6399/8316 (77%)	6324 (99%)	73 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	55	SER

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Mol	Chain	Res	Type
2	w	55	SER

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	0	63/67 (94%)	63 (100%)	0	100	100
1	2	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	3	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	5	63/67 (94%)	63 (100%)	0	100	100
1	6	63/67 (94%)	63 (100%)	0	100	100
1	7	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	8	63/67 (94%)	63 (100%)	0	100	100
1	9	63/67 (94%)	63 (100%)	0	100	100
1	A	63/67 (94%)	63 (100%)	0	100	100
1	A1	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	B	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	C	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	D	63/67 (94%)	63 (100%)	0	100	100
1	E	63/67 (94%)	63 (100%)	0	100	100
1	F	63/67 (94%)	63 (100%)	0	100	100
1	G	63/67 (94%)	63 (100%)	0	100	100
1	H	63/67 (94%)	63 (100%)	0	100	100
1	I	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	J	63/67 (94%)	63 (100%)	0	100	100
1	K	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	L	63/67 (94%)	60 (95%)	3 (5%)	23	57
1	M	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	N	63/67 (94%)	62 (98%)	1 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	P	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	Q	63/67 (94%)	63 (100%)	0	100	100
1	R	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	S	63/67 (94%)	63 (100%)	0	100	100
1	T	63/67 (94%)	63 (100%)	0	100	100
1	U	63/67 (94%)	63 (100%)	0	100	100
1	V	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	W	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	X	63/67 (94%)	63 (100%)	0	100	100
1	Y	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	Z	63/67 (94%)	63 (100%)	0	100	100
1	a	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	b	63/67 (94%)	63 (100%)	0	100	100
1	c	63/67 (94%)	63 (100%)	0	100	100
1	d	63/67 (94%)	63 (100%)	0	100	100
1	e	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	f	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	g	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	h	63/67 (94%)	63 (100%)	0	100	100
1	i	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	j	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	k	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	l	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	m	63/67 (94%)	62 (98%)	1 (2%)	55	79
1	n	63/67 (94%)	63 (100%)	0	100	100
1	o	63/67 (94%)	63 (100%)	0	100	100
1	p	63/67 (94%)	63 (100%)	0	100	100
1	q	63/67 (94%)	63 (100%)	0	100	100
1	r	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	s	63/67 (94%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	t	63/67 (94%)	63 (100%)	0	100	100
1	u	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	v	63/67 (94%)	63 (100%)	0	100	100
2	1	66/67 (98%)	64 (97%)	2 (3%)	36	69
2	4	66/67 (98%)	65 (98%)	1 (2%)	57	80
2	w	66/67 (98%)	65 (98%)	1 (2%)	57	80
2	x	66/67 (98%)	66 (100%)	0	100	100
2	y	66/67 (98%)	64 (97%)	2 (3%)	36	69
2	z	66/67 (98%)	65 (98%)	1 (2%)	57	80
3	A2	95/223 (43%)	94 (99%)	1 (1%)	65	83
3	A3	94/223 (42%)	91 (97%)	3 (3%)	34	67
3	A4	90/223 (40%)	86 (96%)	4 (4%)	25	60
3	A5	92/223 (41%)	90 (98%)	2 (2%)	45	74
3	A6	105/223 (47%)	103 (98%)	2 (2%)	50	76
3	A7	91/223 (41%)	89 (98%)	2 (2%)	45	74
3	X1	38/223 (17%)	37 (97%)	1 (3%)	40	72
3	X2	38/223 (17%)	36 (95%)	2 (5%)	20	54
All	All	4630/6005 (77%)	4570 (99%)	60 (1%)	59	81

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	28	TRP
2	1	81	ASN
1	2	38	ARG
1	2	73	ASP
1	3	27	MET
2	4	28	TRP
1	7	73	ASP
1	7	84	VAL
1	B	66	ASP
1	C	73	ASP
1	I	73	ASP
1	K	73	ASP
1	L	22	GLU
1	L	25	ASP

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Mol	Chain	Res	Type
1	L	73	ASP
1	M	73	ASP
1	N	73	ASP
1	O	73	ASP
1	P	73	ASP
1	R	73	ASP
1	V	73	ASP
1	W	79	HIS
1	Y	22	GLU
1	a	75	LEU
1	e	73	ASP
1	f	73	ASP
1	g	73	ASP
1	i	69	GLU
1	j	53	GLU
1	j	71	VAL
1	k	27	MET
1	k	73	ASP
1	l	73	ASP
1	m	75	LEU
1	r	48	VAL
1	r	49	LEU
1	u	38	ARG
1	u	75	LEU
2	w	10	LEU
2	y	12	SER
2	y	48	ASP
2	z	28	TRP
3	A2	785	VAL
3	A3	791	GLU
3	A3	827	VAL
3	A3	859	SER
3	A4	786	SER
3	A4	809	THR
3	A4	846	SER
3	A4	862	THR
3	A5	862	THR
3	A5	868	ARG
3	A6	862	THR
3	A6	863	TYR
3	A7	780	ASP
3	A7	786	SER

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Mol	Chain	Res	Type
3	X1	624	SER
3	X2	608	SER
3	X2	647	GLN
1	A1	73	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	39	GLN
1	C	58	ASN
1	E	90	ASN
1	H	90	ASN
1	L	58	ASN
1	e	97	GLN
1	n	85	HIS
1	o	97	GLN
1	r	58	ASN
1	v	85	HIS
2	y	14	ASN
3	A2	854	ASN
3	A3	818	ASN
3	A5	781	GLN
3	A5	837	ASN
3	A6	732	HIS
3	A7	781	GLN
3	X1	607	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

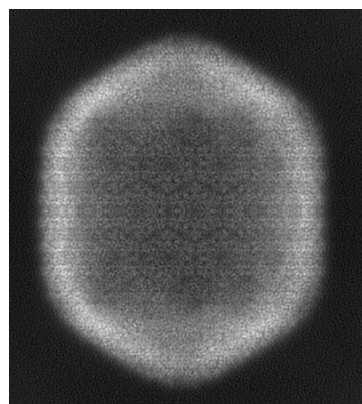
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39599. These allow visual inspection of the internal detail of the map and identification of artifacts.

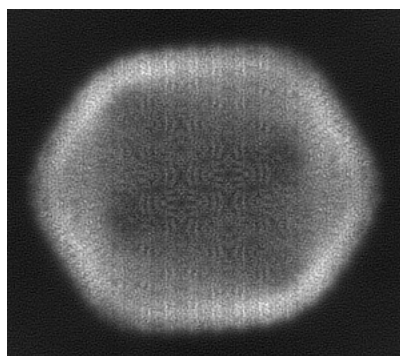
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

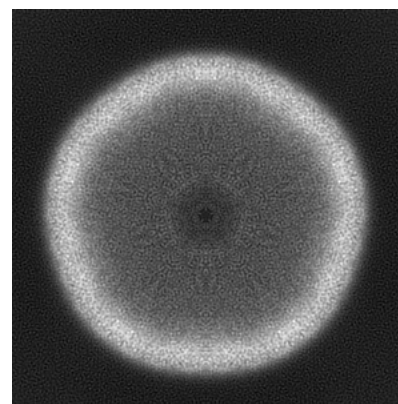
6.1.1 Primary map



X

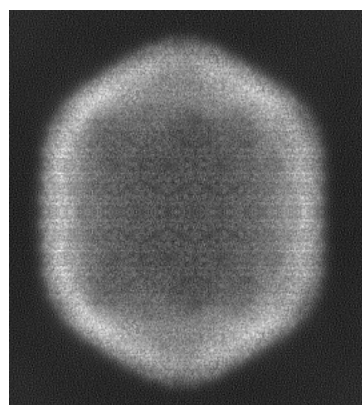


Y

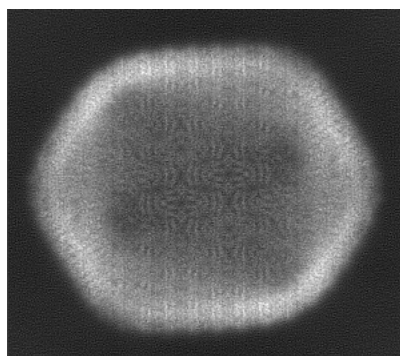


Z

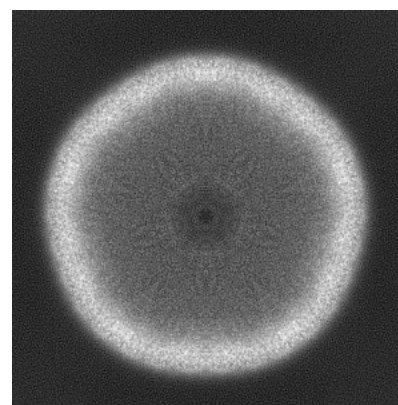
6.1.2 Raw map



X



Y

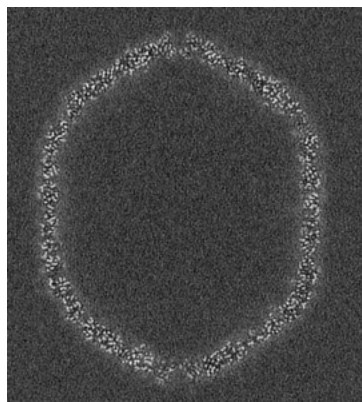


Z

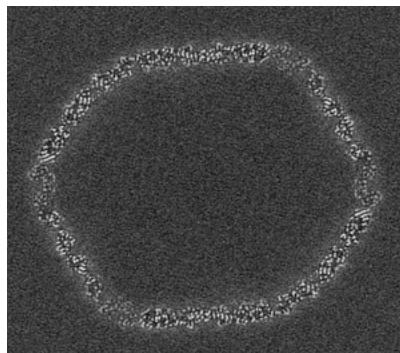
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

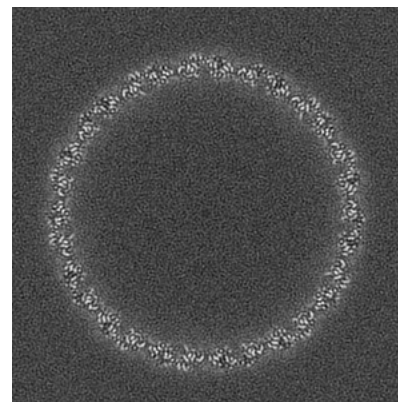
6.2.1 Primary map



X Index: 168

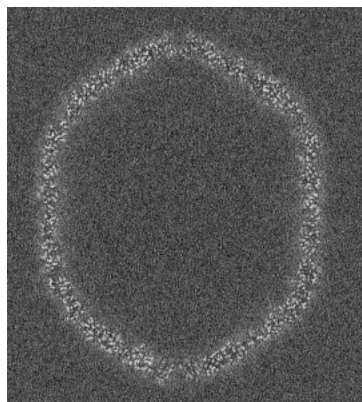


Y Index: 170

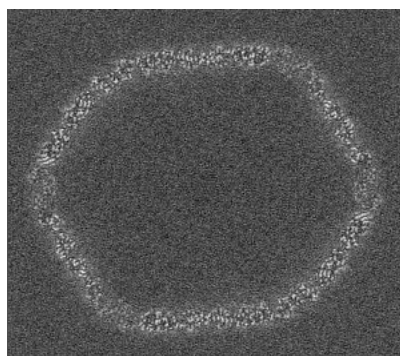


Z Index: 191

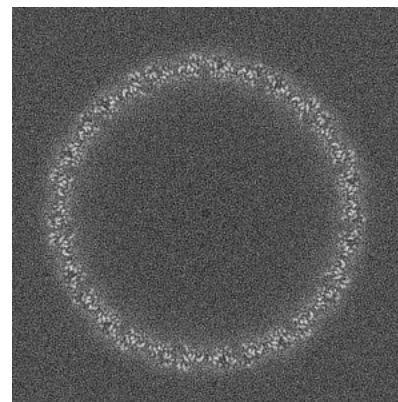
6.2.2 Raw map



X Index: 168



Y Index: 170

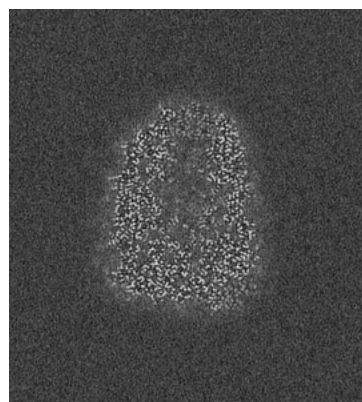


Z Index: 191

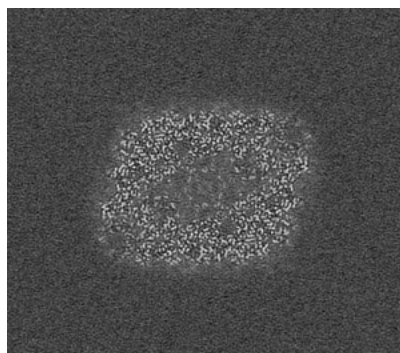
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

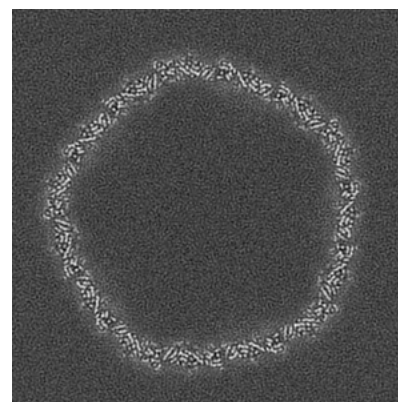
6.3.1 Primary map



X Index: 279

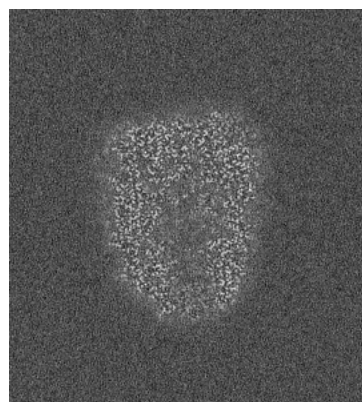


Y Index: 50

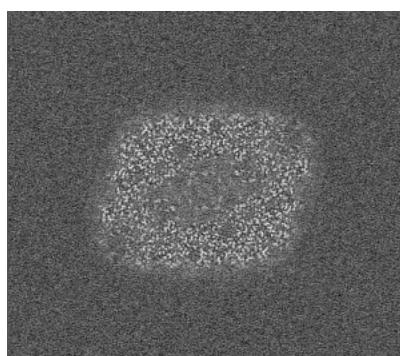


Z Index: 136

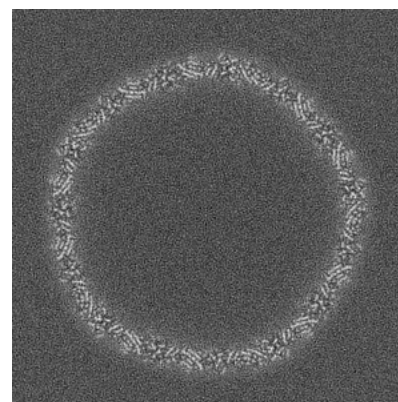
6.3.2 Raw map



X Index: 49



Y Index: 50

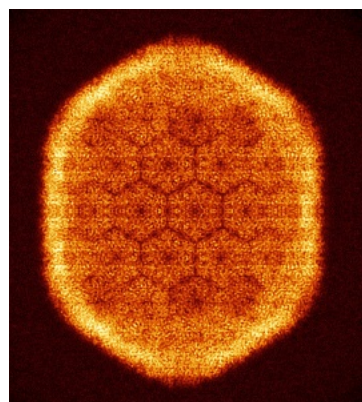


Z Index: 226

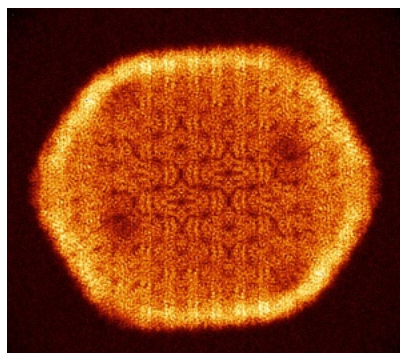
The images above show the largest variance slices of the map in three orthogonal directions.

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

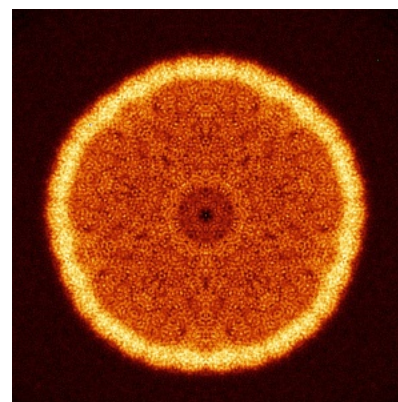
6.4.1 Primary map



X

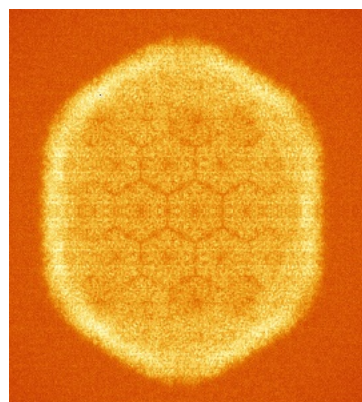


Y

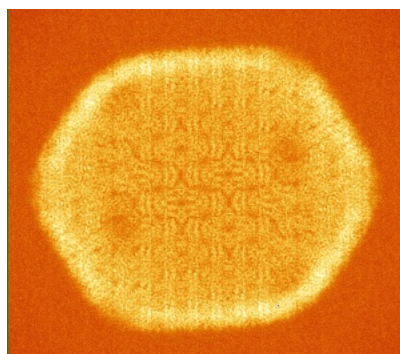


Z

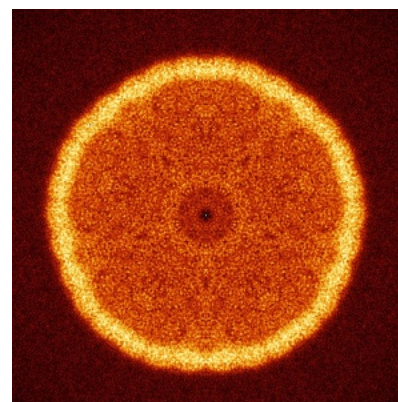
6.4.2 Raw map



X



Y

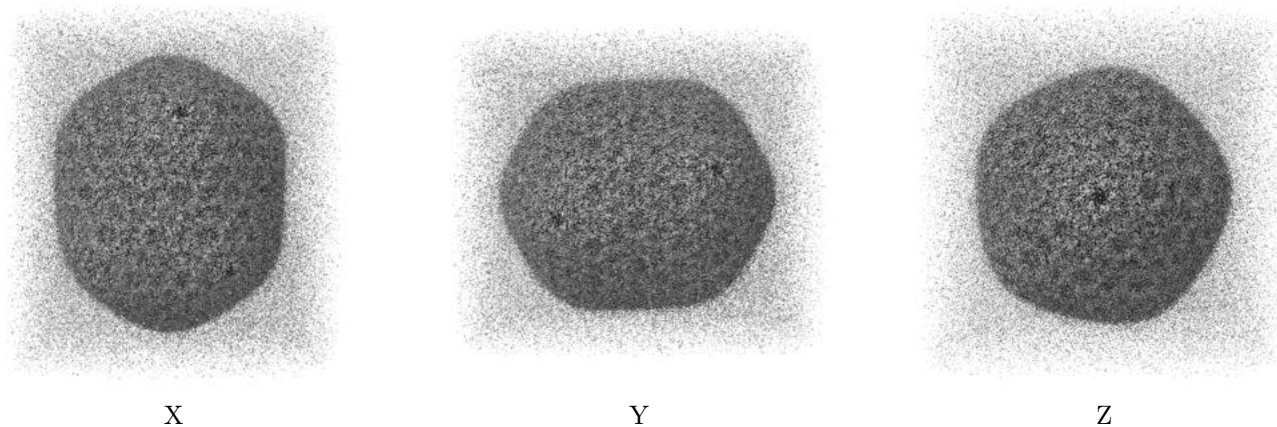


Z

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.

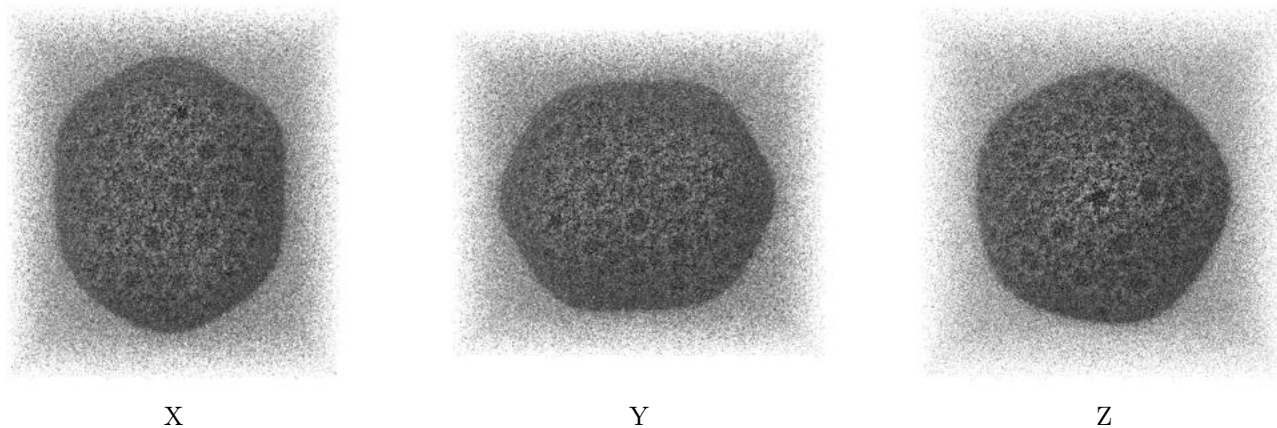
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

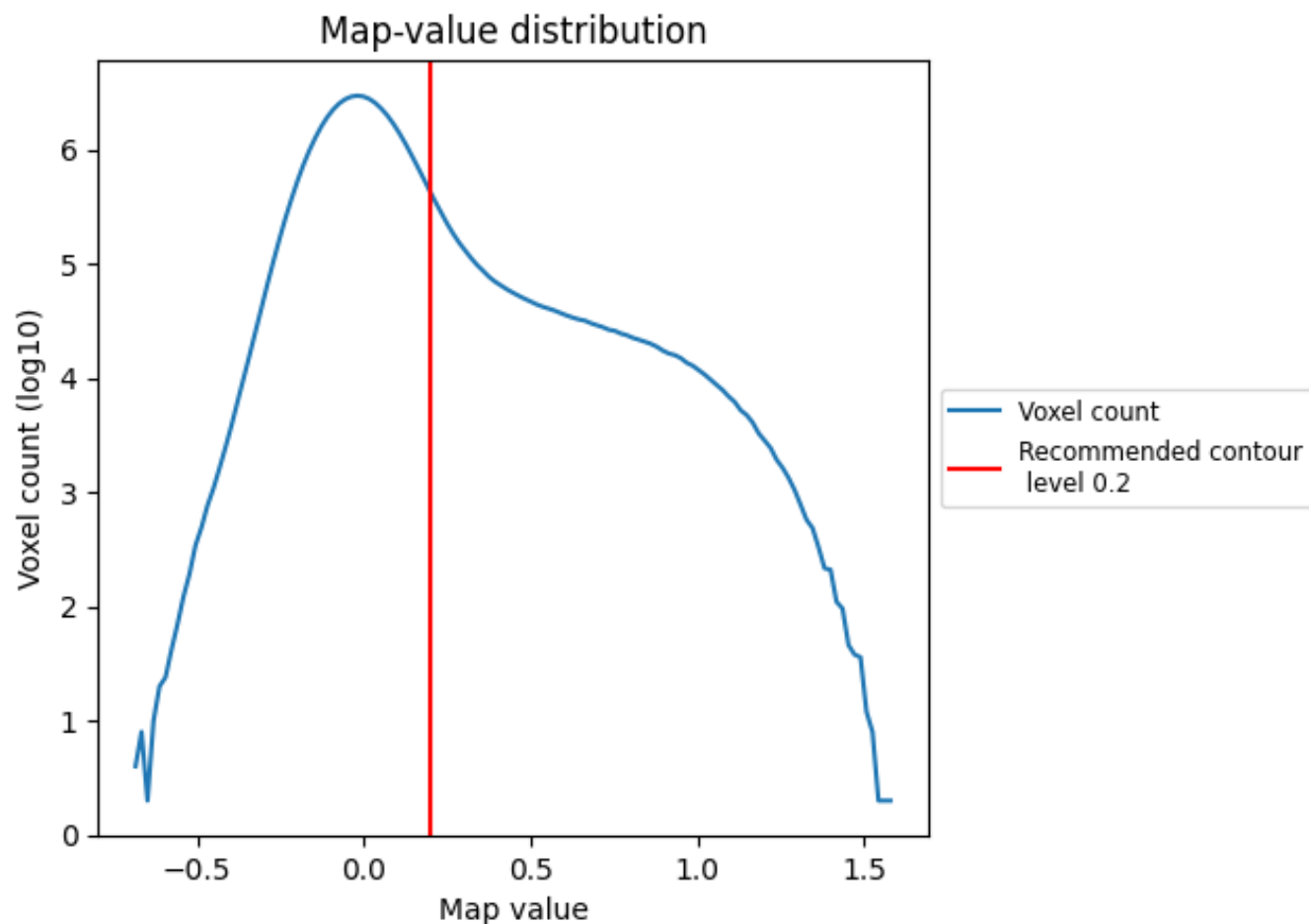
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

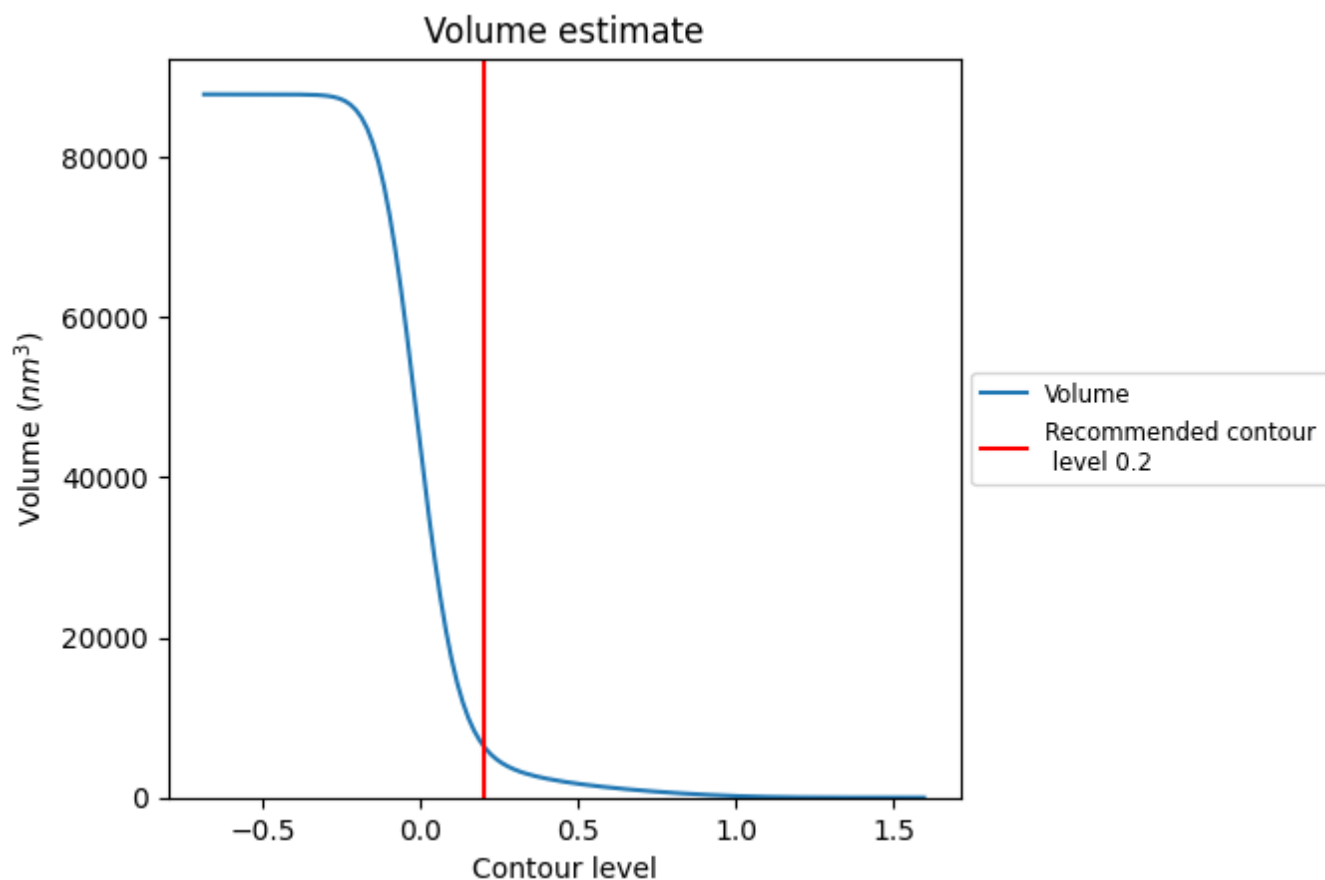
This section contains the results of statistical analysis of the map.

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 6548 nm³; this corresponds to an approximate mass of 5915 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

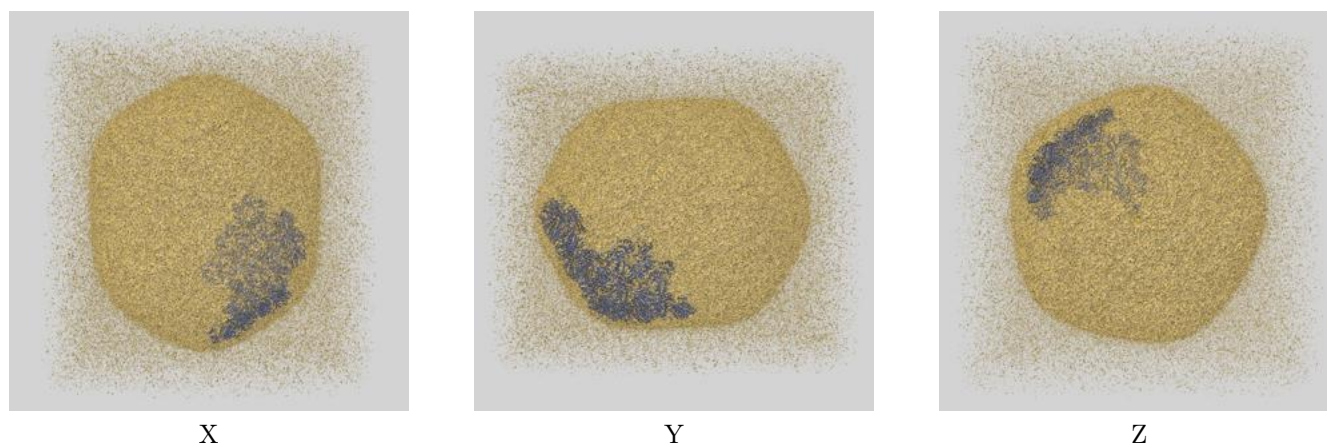
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

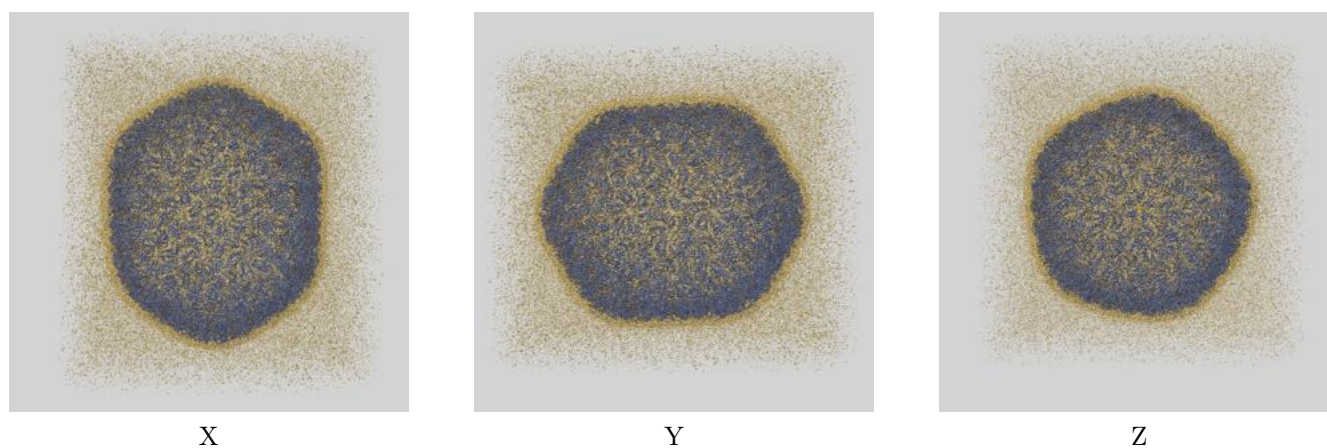
This section contains information regarding the fit between EMDB map EMD-39599 and PDB model 8YVF. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

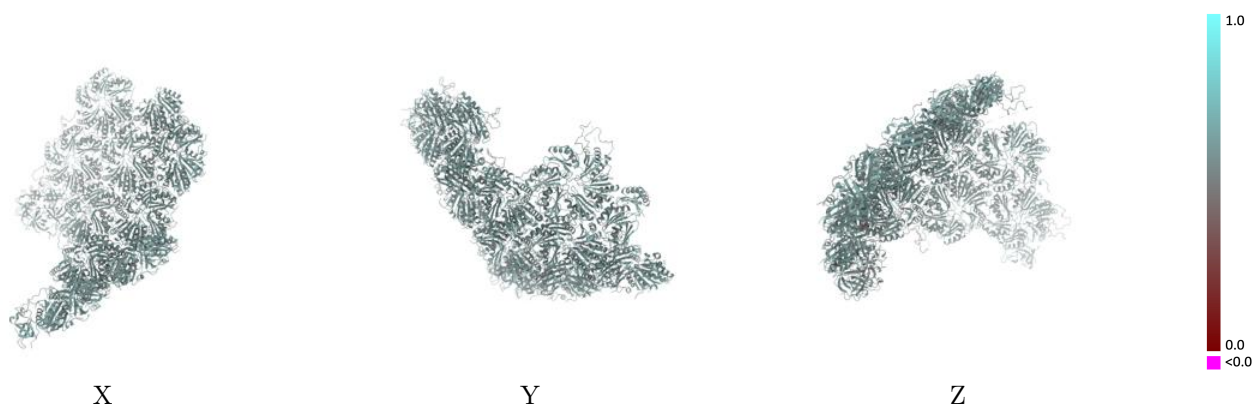


9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 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](#)

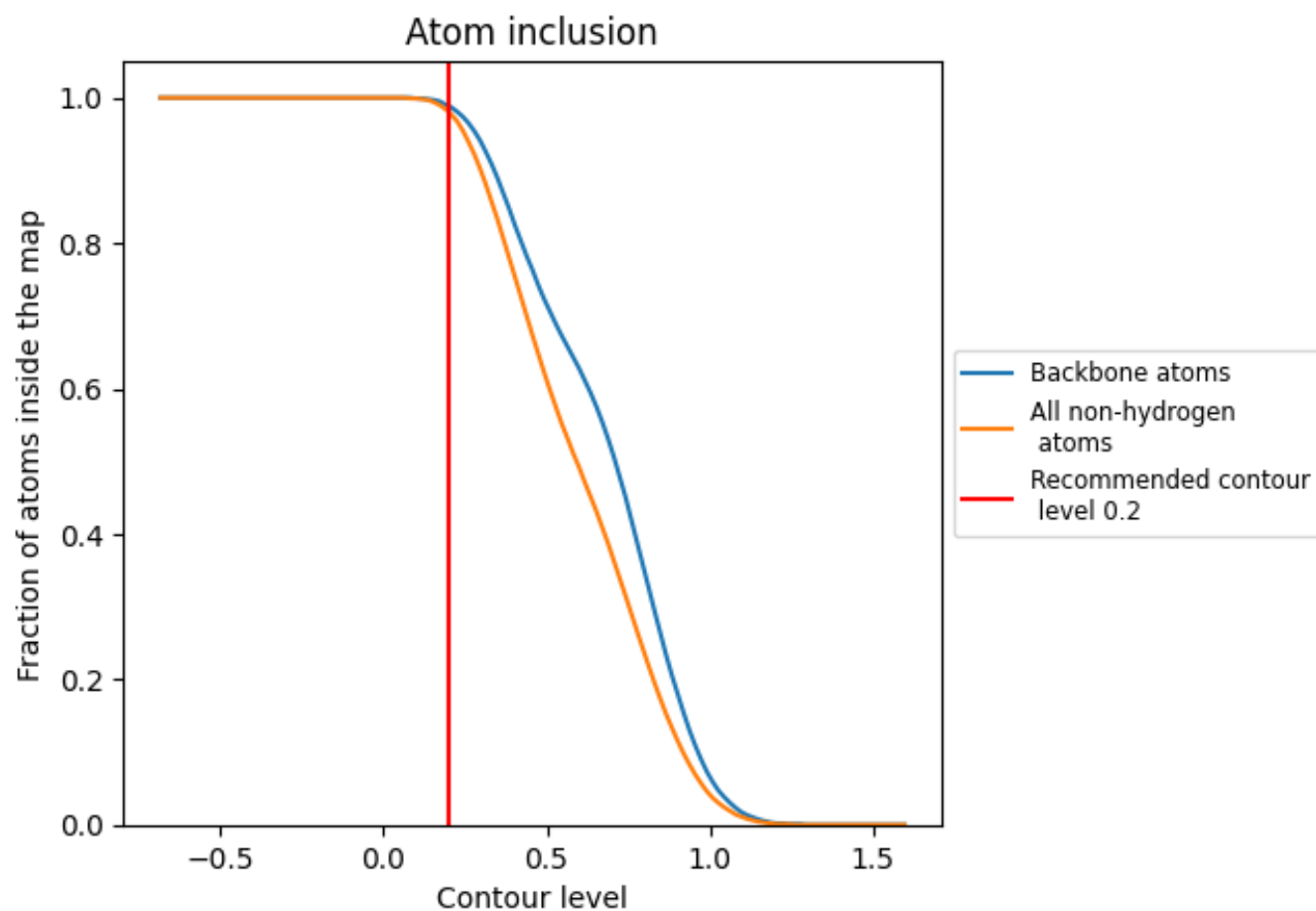


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.5690
0	 0.9810	 0.5710
1	 0.9570	 0.5590
2	 0.9890	 0.5760
3	 0.9880	 0.5720
4	 0.9630	 0.5640
5	 0.9890	 0.5750
6	 0.9910	 0.5740
7	 0.9950	 0.5800
8	 0.9910	 0.5790
9	 0.9910	 0.5690
A	 0.9860	 0.5770
A1	 0.9840	 0.5740
A2	 0.9320	 0.5410
A3	 0.9510	 0.5340
A4	 0.9480	 0.5330
A5	 0.9680	 0.5420
A6	 0.9480	 0.5330
A7	 0.9390	 0.5190
B	 0.9840	 0.5770
C	 0.9940	 0.5820
D	 0.9940	 0.5800
E	 0.9940	 0.5760
F	 0.9940	 0.5880
G	 0.9910	 0.5740
H	 0.9970	 0.5820
I	 0.9880	 0.5790
J	 0.9940	 0.5790
K	 0.9860	 0.5740
L	 0.9880	 0.5780
M	 0.9810	 0.5760
N	 0.9950	 0.5720
O	 0.9970	 0.5750
P	 0.9970	 0.5740
Q	 0.9860	 0.5880



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Chain	Atom inclusion	Q-score
R	 0.9880	 0.5820
S	 0.9940	 0.5730
T	 0.9920	 0.5770
U	 0.9770	 0.5710
V	 0.9910	 0.5790
W	 0.9950	 0.5730
X	 0.9920	 0.5770
X1	 0.9410	 0.5290
X2	 0.9520	 0.5390
Y	 0.9780	 0.5680
Z	 0.9890	 0.5810
a	 0.9860	 0.5710
b	 0.9920	 0.5750
c	 0.9860	 0.5750
d	 0.9880	 0.5810
e	 0.9890	 0.5710
f	 0.9950	 0.5780
g	 0.9940	 0.5780
h	 0.9880	 0.5750
i	 0.9880	 0.5740
j	 0.9920	 0.5760
k	 0.9950	 0.5720
l	 0.9810	 0.5710
m	 0.9880	 0.5720
n	 0.9910	 0.5740
o	 0.9880	 0.5730
p	 0.9910	 0.5740
q	 0.9980	 0.5780
r	 0.9950	 0.5740
s	 0.9950	 0.5760
t	 0.9860	 0.5710
u	 0.9910	 0.5790
v	 0.9810	 0.5660
w	 0.9250	 0.5490
x	 0.9430	 0.5490
y	 0.9350	 0.5560
z	 0.9300	 0.5480