



Full wwPDB EM Validation Report ⓘ

Mar 13, 2026 – 11:30 AM UTC

PDB ID : 8AFH / pdb_00008afh
EMDB ID : EMD-15398
Title : Cryo-EM structure of crescentin filaments (stutter mutant, C2, symmetry and small box)
Authors : Liu, Y.; Lowe, J.
Deposited on : 2022-07-18
Resolution : 3.90 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

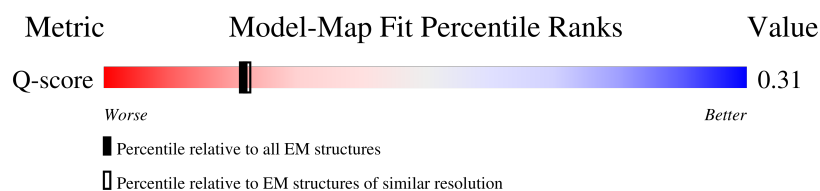
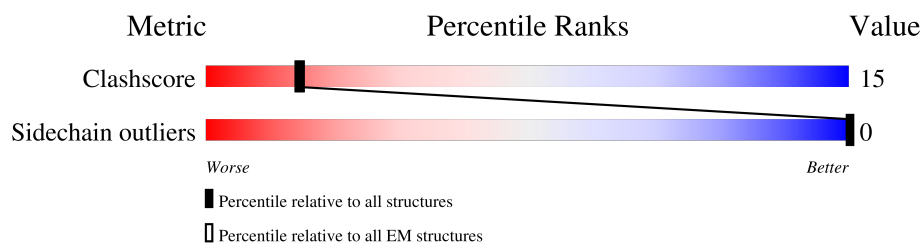
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



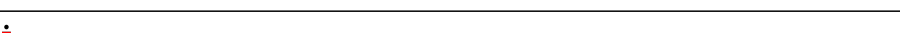
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	460	
1	B	460	
1	E	460	
1	F	460	
1	G	460	

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Mol	Chain	Length	Quality of chain
1	H	460	 7% 92%
1	K	460	 17% 79%
1	L	460	 15% 6% 79%
1	O	460	 14% 83%
1	P	460	 15% 83%
1	Q	460	 7% 91%
1	R	460	 7% 92%
2	C	907	 8% 5% 88%
2	D	907	 8% 5% 88%
2	I	907	 8% 88%
2	J	907	 8% 5% 88%
2	M	907	 7% 5% 88%
2	N	907	 8% 5% 88%
2	S	907	 8% 88%
2	T	907	 8% 88%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13570 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 Crescentin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	96	Total	C	N	O	S	0	0
			739	438	152	148	1		
1	B	97	Total	C	N	O	S	0	0
			747	443	153	149	2		
1	E	79	Total	C	N	O		0	0
			600	359	114	127			
1	F	79	Total	C	N	O		0	0
			600	359	114	127			
1	G	43	Total	C	N	O		0	0
			333	197	69	67			
1	H	39	Total	C	N	O		0	0
			299	177	61	61			
1	K	96	Total	C	N	O	S	0	0
			739	438	152	148	1		
1	L	97	Total	C	N	O	S	0	0
			747	443	153	149	2		
1	O	79	Total	C	N	O		0	0
			600	359	114	127			
1	P	79	Total	C	N	O		0	0
			600	359	114	127			
1	Q	43	Total	C	N	O		0	0
			333	197	69	67			
1	R	39	Total	C	N	O		0	0
			299	177	61	61			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP A0A8F8EC09
A	407	ALA	-	insertion	UNP A0A8F8EC09
A	408	THR	-	insertion	UNP A0A8F8EC09
B	406	SER	-	insertion	UNP A0A8F8EC09
B	407	ALA	-	insertion	UNP A0A8F8EC09
B	408	THR	-	insertion	UNP A0A8F8EC09

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Chain	Residue	Modelled	Actual	Comment	Reference
E	406	SER	-	insertion	UNP A0A8F8EC09
E	407	ALA	-	insertion	UNP A0A8F8EC09
E	408	THR	-	insertion	UNP A0A8F8EC09
F	406	SER	-	insertion	UNP A0A8F8EC09
F	407	ALA	-	insertion	UNP A0A8F8EC09
F	408	THR	-	insertion	UNP A0A8F8EC09
G	406	SER	-	insertion	UNP A0A8F8EC09
G	407	ALA	-	insertion	UNP A0A8F8EC09
G	408	THR	-	insertion	UNP A0A8F8EC09
H	406	SER	-	insertion	UNP A0A8F8EC09
H	407	ALA	-	insertion	UNP A0A8F8EC09
H	408	THR	-	insertion	UNP A0A8F8EC09
K	406	SER	-	insertion	UNP A0A8F8EC09
K	407	ALA	-	insertion	UNP A0A8F8EC09
K	408	THR	-	insertion	UNP A0A8F8EC09
L	406	SER	-	insertion	UNP A0A8F8EC09
L	407	ALA	-	insertion	UNP A0A8F8EC09
L	408	THR	-	insertion	UNP A0A8F8EC09
O	406	SER	-	insertion	UNP A0A8F8EC09
O	407	ALA	-	insertion	UNP A0A8F8EC09
O	408	THR	-	insertion	UNP A0A8F8EC09
P	406	SER	-	insertion	UNP A0A8F8EC09
P	407	ALA	-	insertion	UNP A0A8F8EC09
P	408	THR	-	insertion	UNP A0A8F8EC09
Q	406	SER	-	insertion	UNP A0A8F8EC09
Q	407	ALA	-	insertion	UNP A0A8F8EC09
Q	408	THR	-	insertion	UNP A0A8F8EC09
R	406	SER	-	insertion	UNP A0A8F8EC09
R	407	ALA	-	insertion	UNP A0A8F8EC09
R	408	THR	-	insertion	UNP A0A8F8EC09

- Molecule 2 is a protein called Crescentus-specific megabody MB13.

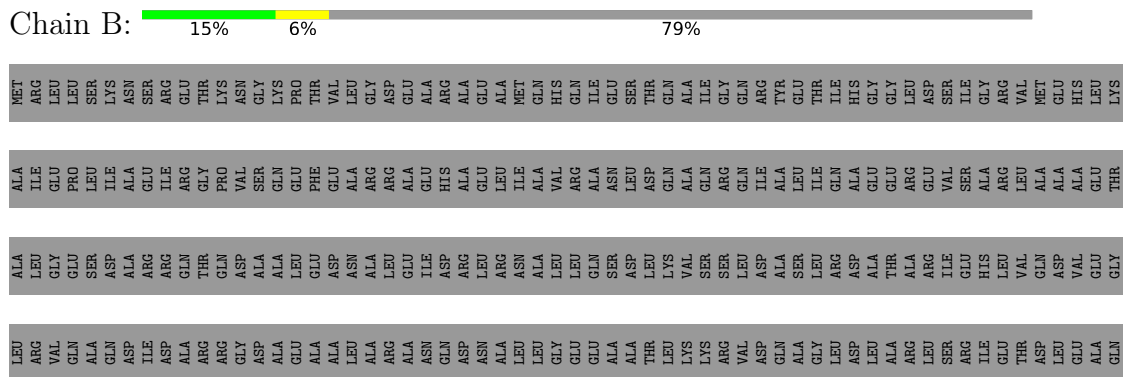
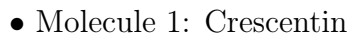
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	C	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	I	111	Total	C	N	O	S	0	0
			860	534	154	167	5		
2	J	112	Total	C	N	O	S	0	0
			869	539	155	170	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	112	Total 869	C 539	N 155	O 170	S 5	0	0
2	M	112	Total 869	C 539	N 155	O 170	S 5	0	0
2	S	111	Total 860	C 534	N 154	O 167	S 5	0	0
2	T	112	Total 869	C 539	N 155	O 170	S 5	0	0

- Molecule 1: Crescentin





[illegible]

- Molecule 1: Crescentin

Chain G: 7% . 91%

[illegible]

A433 Q445

MET	ALA
LEU	LEU
GLY	ALA
SER	SER
ASP	GLY
ASP	VAL
ALA	ALA
SER	ALA

- Molecule 1: Crescentin

Chain H: 7% . 92%

[illegible]

R441	SER
	ARG
	LEU
	GLN
	MET
	ALA
	LEU
	LEU
	GLY
	ALA
	SER
	ASP
	GLY
	ASP
	VAL
	ALA
	ALA
	SER
	ALA

Chain K: 17% 79%

LEU	ALA	ALA	GLU	ARG	ARG	ALA	VAL	GLN	ALA	ALA	VAL	GLU	ASN	ALA	LEU	ALA	ALA	HIS	GLN	ASP	SER	GLY	THR	ILE	ARG	GLY	LEU	GLU	SER	GLN	VAL	GLU	ALA	ASN	ARG	ALA	GLU	THR	ARG	GLY	GLY	THR	LEU	ASP	LYS	LEU	GLU	GLU	NEP
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R363	A364	D365	D366	L367	L368	K369	S370	A373	L378	K379	R380	R391	M395	A398	L416	Q417	A418	T419	I420	E426	A427	A428	L434	R438	R443	L444	Q445	Q45	ALA	LEU	LEU	GLY	ALA	GLY	SER	ASP	GLY	ASP	VAL	ALA	ALA	ALA	SER	ALA
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Chain L: 15% 6% 79%

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



GLN	ALA	THR	ILE	GLU	ARG	LEU	THR	SER	GLU	ALA	ALA	LEU	ALA	GLU	GLY	ALA	LEU	GLU	ALA	ARG	ARG	ASP	ARG	SER	ARG	LEU	GLN	MET	ALA	LEU	LEU	GLY	ALA	SER	ASP	GLY	ASP	VAL	ALA	ALA	ALA	SER	ALA
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- Molecule 1: Crescentin

Chain Q: 7% 91%

ALA LEU GLY SER ASP ALA ARG ARG GLN THR GLN ASP ALA ALA LEU GLU GLU ASN ASN LEU LEU LYS VAL SER SER LEU LEU ASP ALA SER LEU LEU ASP ARG THR ALA ARG ILE GLU HIS LEU VAL GLN ASP VAL GLY

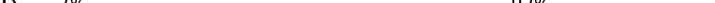
LEU ARG VAL GLN GLN ASP ASP ASP ASP ARG ARG GLY ASP ASP GLU GLU ALA ALA ALA LEU LEU ARG ALA ALA ASN ASN ASP GLN GLY GLU GLU ALA ALA ALA THR THR LEU LEU LYS LYS ARG ARG VAL VAL ASP ASP GLN GLY GLY ALA LEU LEU LYS LYS ARG ARG ASP ASP ALA ALA ARG ARG SER SER LEU LEU LEU LEU GLU GLU THR THR GLU GLN ALA

LEU
ALA
ALA
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ARG
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ASN
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HIS
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ASP
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GLY
ALA
ASP
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LEU
LEU
GLU
GLU
THR

ASN	GLN	GLY	ILE	SER	ALA	ARG	LEU	ALA	ASP	SER	SER	ALA	GLN	LYS	VAL	GLU	ARG	ARG	ALA	GLY	ASP	LEU	ASN	VAL	ALA	ALA	LEU	GLU	ARG	ALA	LEU	ASP	ARG	ILE	ARG	ALA	LEU	GLU	GLU	ALA	ASP	GLY	LEU	LEU	ARG	ARG	GLN	ARG	HIS	ALA	GLY	VAL	ASP	THR	ALA	ALA	THR	ALA
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TLE	GLU	ARG	ALA	ASP	GLN	LEU	ALA	LYS	SER	VAL	ALA	GLN	GLU	LYS	ALA	LEU	LYS	ARG	ALA	GLU	GLU	ARG	ALA	GLN	GLN	LEU	ARG	ASP	ALA	MET	GLN	GLU	ALA	GLN	ASP	GLN	VAL	R403	R404	D405	S406	A407	T408	H409	Q417	E421	R422	L423	T424	S425	E431
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- Molecule 1: Crescentin

Chain R:  7% 92%

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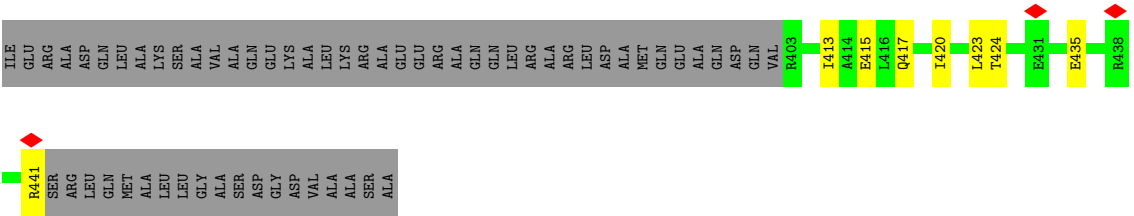
ALA	TLE	GLU	PRO	LEU	TLE	ALA	GLU	ARG	GLY	VAL	PRO	SER	GLN	GLU	PHE	ALA	ALA	ARG	ARG	GLU	HIS	ALA	GLU	LEU	TLE	ALA	VAL	ARG	ASN	GLN	ASP	LEU	LEU	GLN	ALA	ALA	TLE	ALA	LEU	TLE	GLN	GLN	GLU	VAL	ARG	GLU	LEU	ALA	ALA	ALA	ALA	ALA	GLU	THR
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ALA	LEU	GLY	GLU	SER	ASP	ALA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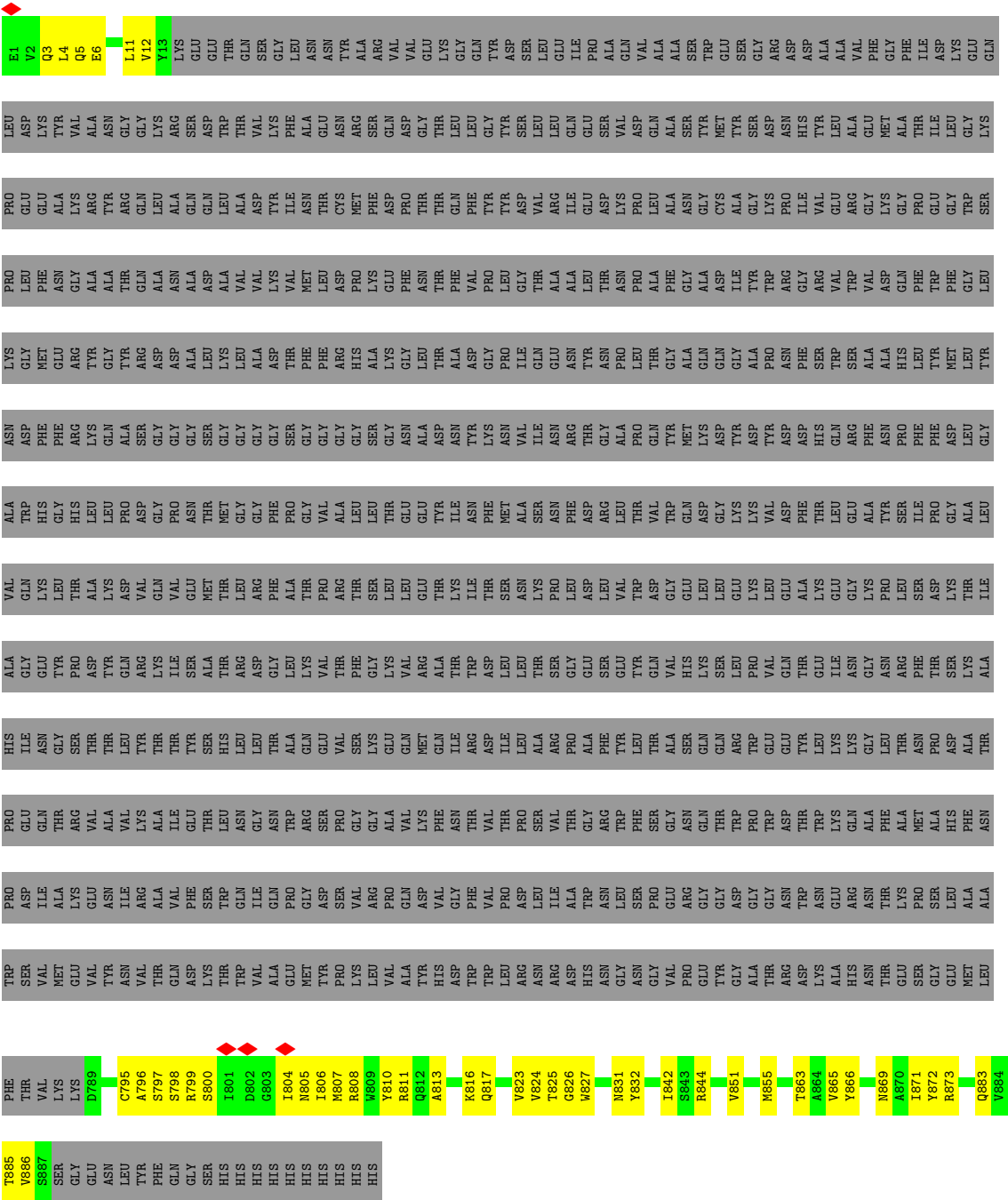
AB
LEU ARG VAL ALA GLN GLY ASP ASN ASP ASP ARG ARG GLY LEU LEU LEU LEU THR LYS LYS ARG ASP VAL ASP GLN GLY GLY LEU LEU LEU LEU SER SER THR ASP LEU LEU GYL ALA GLN

LEU
ALA
ALA
GLU
ARG
ARG
VAL
GLN
ALA
VAL
GLU
ASN
ALA
ALA
ALA
HIS
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ARG
ALA
ASP
LYS
LEU
GLU
GLU
MET

	ASN	GNY	GLN	TLE	SER	ALA	ARG	LEU	ASP	SER	SER	ALA	GLN	LYS	VAL	GLU	ARG	ASN	VAL	ALA	LEU	GLU	ARG	TLE	ARG	ALA	LEU	GLU	GLU	GLU	ALA	ASP	GLY	LEU	GLU	ARG	GLN	ARG	HIS	ALA	GLY	VAL	ASP	THR	ALA	ALA	ALA	THR	THR	ALA	ALA	ALA
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• Molecule 2: Crescentus-specific megabody MB13



[illegible]

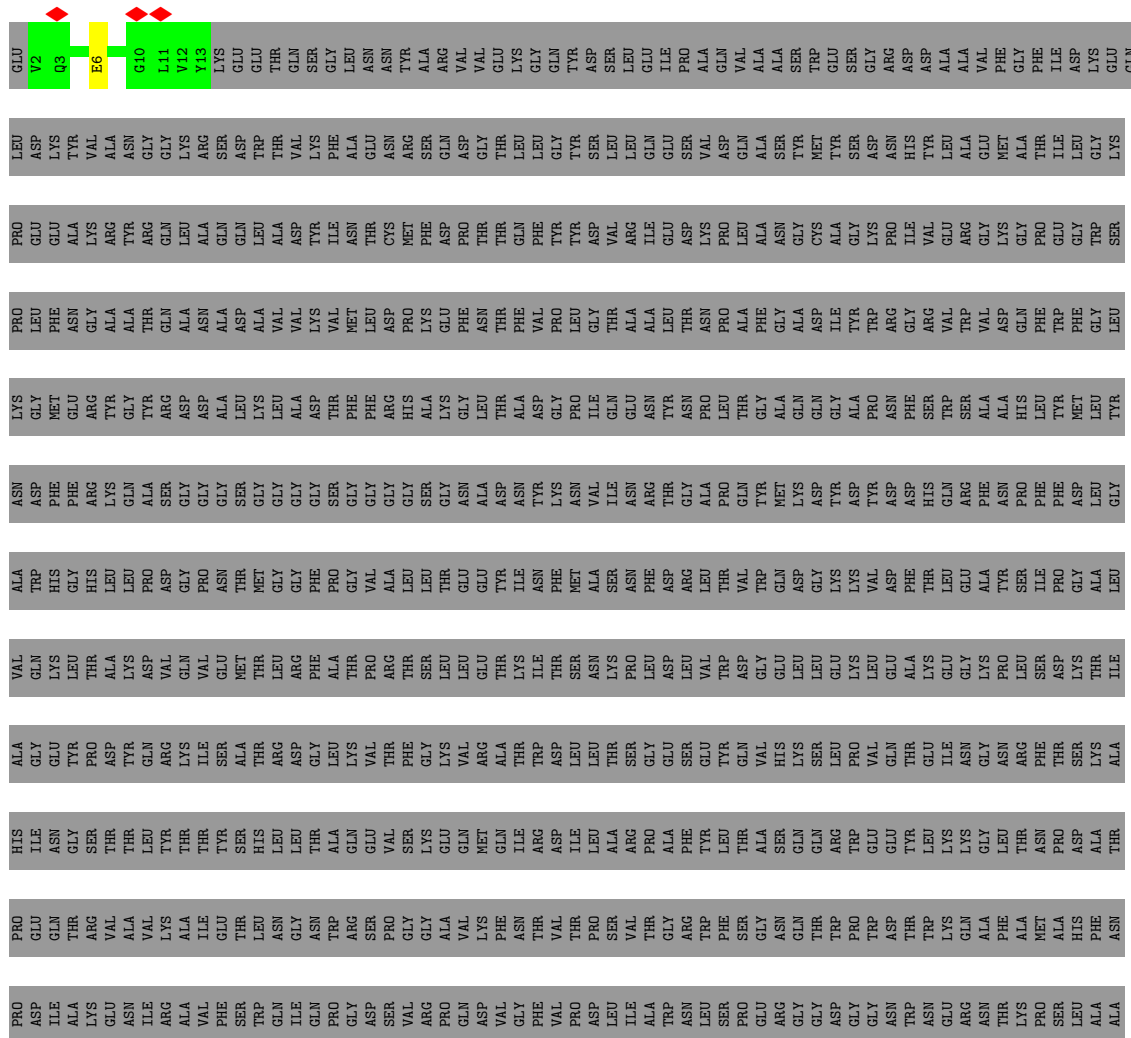
GLU	V2	E6	V13	LYS	GLU	GLU	GLU	THR	GLN	GLN	GLY	LEU	ASN	ASN	TYR	ALA	ALA	ARG	VAL	VAL	GLU	GLY	GLN	TYR	ASP	SER	LEU	LEU	ILE	ILE	PRO	ALA	GLN	VAL	VAL	ALA	ALA	ALA	SER	SER	ASP	ASP	TRP	GLU	SER	SER	GLY	GLY	ARG	ASP	GLY	PHE	PHE	ILE	ILE	ASP	LYS	GLY	GLN	LEU	ASP	LYS	TYR
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[illegible]

Chain M: 7% 5% 88%









Q880	G881	T882	Q883	V884	T885	V886	S887	SER	GLY	GLU	ASN	LEU	TYR	PHE	GLN	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	599993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.996	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	424.0, 424.0, 424.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.325, 1.325, 1.325	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	0.21	0/740	0.42	0/991
1	B	0.23	0/748	0.44	0/1001
1	E	0.28	0/599	0.53	0/808
1	F	0.27	0/599	0.45	0/808
1	G	0.23	0/333	0.43	0/445
1	H	0.26	0/299	0.50	0/400
1	K	0.21	0/740	0.42	0/991
1	L	0.23	0/748	0.44	0/1001
1	O	0.28	0/599	0.52	0/808
1	P	0.27	0/599	0.45	0/808
1	Q	0.23	0/333	0.43	0/445
1	R	0.25	0/299	0.50	0/400
2	C	0.31	0/883	0.45	0/1192
2	D	0.30	0/883	0.44	0/1192
2	I	0.29	0/874	0.44	0/1180
2	J	0.28	0/883	0.43	0/1192
2	M	0.32	0/883	0.45	0/1192
2	N	0.30	0/883	0.44	0/1192
2	S	0.29	0/874	0.44	0/1180
2	T	0.28	0/883	0.43	0/1192
All	All	0.27	0/13682	0.45	0/18418

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	739	0	745	29	0
1	B	747	0	754	30	0
1	E	600	0	601	17	0
1	F	600	0	601	13	0
1	G	333	0	336	10	0
1	H	299	0	299	13	0
1	K	739	0	745	30	0
1	L	747	0	754	31	0
1	O	600	0	601	16	0
1	P	600	0	601	12	0
1	Q	333	0	336	10	0
1	R	299	0	299	12	0
2	C	869	0	846	36	0
2	D	869	0	846	52	0
2	I	860	0	837	29	0
2	J	869	0	846	33	0
2	M	869	0	846	37	0
2	N	869	0	846	50	0
2	S	860	0	837	29	0
2	T	869	0	846	32	0
All	All	13570	0	13422	409	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 15.

All (409) 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:D:873:ARG:HE	1:L:396:GLN:CD	1.69	1.00
1:B:396:GLN:CD	2:N:873:ARG:HE	1.70	1.00
1:H:441:ARG:NH2	1:K:358:ALA:CB	2.28	0.97
1:H:441:ARG:NH2	1:K:358:ALA:HB2	1.83	0.92
2:M:808:ARG:HG2	2:M:823:VAL:HG22	1.52	0.92
2:C:808:ARG:HG2	2:C:823:VAL:HG22	1.52	0.90
2:D:873:ARG:NE	1:L:396:GLN:CD	2.30	0.89
1:H:441:ARG:HH22	1:K:358:ALA:HB2	1.38	0.86
1:B:396:GLN:CD	2:N:873:ARG:NE	2.32	0.85
1:A:358:ALA:CB	1:R:441:ARG:NH2	2.40	0.84
2:D:873:ARG:HE	1:L:396:GLN:NE2	1.74	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLN:NE2	2:N:873:ARG:HE	1.77	0.82
1:A:358:ALA:HB2	1:R:441:ARG:NH2	1.97	0.80
1:B:424:THR:O	2:C:831:ASN:ND2	2.16	0.79
1:L:424:THR:O	2:M:831:ASN:ND2	2.16	0.79
2:S:808:ARG:HG2	2:S:823:VAL:HG22	1.66	0.78
2:I:808:ARG:HG2	2:I:823:VAL:HG22	1.66	0.78
2:J:4:LEU:HD11	2:J:870:ALA:HB2	1.67	0.77
1:K:438:ARG:HH12	2:N:817:GLN:HB2	1.48	0.76
1:A:438:ARG:HH12	2:D:817:GLN:HB2	1.48	0.75
2:T:4:LEU:HD11	2:T:870:ALA:HB2	1.67	0.75
1:A:358:ALA:HB2	1:R:441:ARG:HH22	1.51	0.75
2:D:799:ARG:NH1	2:D:800:SER:OG	2.20	0.75
2:N:799:ARG:NH1	2:N:800:SER:OG	2.20	0.74
2:D:873:ARG:HD3	1:L:396:GLN:OE1	1.87	0.73
2:T:808:ARG:HB3	2:T:823:VAL:HG12	1.71	0.71
1:B:396:GLN:OE1	2:N:873:ARG:HD3	1.91	0.70
1:O:111:VAL:HG22	1:O:115:LEU:HD12	1.73	0.70
2:I:802:ASP:OD1	2:I:844:ARG:NH2	2.25	0.70
2:S:808:ARG:NH2	2:S:810:TYR:OH	2.25	0.70
2:J:808:ARG:HB3	2:J:823:VAL:HG12	1.71	0.70
2:I:808:ARG:NH2	2:I:810:TYR:OH	2.25	0.70
1:E:111:VAL:HG22	1:E:115:LEU:HD12	1.73	0.69
2:S:802:ASP:OD1	2:S:844:ARG:NH2	2.25	0.69
1:H:441:ARG:HH22	1:K:358:ALA:CB	1.99	0.68
1:L:400:ASP:O	1:L:404:ARG:NH1	2.28	0.67
2:N:808:ARG:HE	2:N:869:ASN:HD22	1.43	0.67
2:D:808:ARG:HE	2:D:869:ASN:HD22	1.43	0.67
1:B:400:ASP:O	1:B:404:ARG:NH1	2.28	0.66
2:J:855:MET:HB3	2:J:858:LEU:HD21	1.78	0.66
1:O:115:LEU:HD11	1:P:111:VAL:HG13	1.79	0.65
2:C:805:ASN:H	2:C:872:TYR:HE1	1.45	0.64
1:E:115:LEU:HD11	1:F:111:VAL:HG13	1.79	0.64
2:T:855:MET:HB3	2:T:858:LEU:HD21	1.78	0.64
2:C:844:ARG:NH2	2:C:846:SER:OG	2.31	0.64
1:H:441:ARG:NH2	1:K:358:ALA:HB1	2.13	0.63
2:I:811:ARG:NH1	2:I:862:ASP:OD1	2.29	0.63
1:L:413:ILE:O	1:L:417:GLN:HG3	1.99	0.63
2:M:844:ARG:NH2	2:M:846:SER:OG	2.31	0.63
1:B:415:GLU:OE1	2:D:805:ASN:ND2	2.32	0.63
2:S:811:ARG:NH1	2:S:862:ASP:OD1	2.28	0.63
1:B:413:ILE:O	1:B:417:GLN:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:805:ASN:H	2:M:872:TYR:HE1	1.46	0.62
2:S:792:ARG:NE	2:S:854:GLN:OE1	2.32	0.62
1:A:358:ALA:CB	1:R:441:ARG:HH22	2.09	0.62
2:I:792:ARG:NE	2:I:854:GLN:OE1	2.32	0.61
1:L:415:GLU:OE1	2:N:805:ASN:ND2	2.32	0.61
1:E:129:ARG:NH2	1:F:125:SER:O	2.34	0.60
2:N:6:GLU:OE1	2:N:6:GLU:N	2.35	0.60
2:D:6:GLU:N	2:D:6:GLU:OE1	2.35	0.59
2:I:822:ALA:HB1	2:I:842:ILE:HB	1.85	0.59
1:O:129:ARG:NH2	1:P:125:SER:O	2.34	0.59
2:N:795:CYS:HB3	2:N:851:VAL:HG12	1.84	0.59
1:A:417:GLN:HE21	2:D:827:TRP:CD1	2.21	0.59
2:T:869:ASN:OD1	2:T:870:ALA:N	2.36	0.58
2:S:822:ALA:HB1	2:S:842:ILE:HB	1.85	0.58
2:J:869:ASN:OD1	2:J:870:ALA:N	2.36	0.58
2:J:866:TYR:N	2:J:882:THR:O	2.31	0.58
2:N:808:ARG:HG3	2:N:810:TYR:HE1	1.69	0.58
2:T:866:TYR:N	2:T:882:THR:O	2.31	0.58
2:D:873:ARG:CD	1:L:396:GLN:OE1	2.52	0.58
2:D:795:CYS:HB3	2:D:851:VAL:HG12	1.84	0.58
1:O:115:LEU:HD22	1:P:114:ARG:HH11	1.69	0.58
2:C:863:THR:HG23	2:C:885:THR:HA	1.86	0.58
2:C:824:VAL:HG23	2:C:830:THR:HG22	1.86	0.57
2:D:826:GLY:O	2:D:844:ARG:NH1	2.37	0.57
2:M:824:VAL:HG23	2:M:830:THR:HG22	1.86	0.57
1:H:417:GLN:O	1:H:420:ILE:HG22	2.04	0.57
1:R:417:GLN:O	1:R:420:ILE:HG22	2.04	0.57
2:D:808:ARG:HG3	2:D:810:TYR:HE1	1.69	0.57
2:N:863:THR:HG23	2:N:885:THR:HA	1.87	0.57
1:L:362:GLU:HA	1:L:365:ASP:HB2	1.87	0.56
2:M:863:THR:HG23	2:M:885:THR:HA	1.86	0.56
2:C:832:TYR:HB2	2:C:837:LYS:HG2	1.86	0.56
1:K:417:GLN:HE21	2:N:827:TRP:CD1	2.21	0.56
1:L:425:SER:HA	2:M:831:ASN:HD22	1.70	0.56
2:M:832:TYR:HB2	2:M:837:LYS:HG2	1.86	0.56
2:M:869:ASN:ND2	2:M:876:GLU:OE2	2.38	0.56
1:H:413:ILE:HG22	2:I:827:TRP:HZ2	1.71	0.56
2:S:841:ILE:HB	2:S:854:GLN:HB3	1.88	0.56
1:A:358:ALA:HB1	1:R:441:ARG:NH2	2.21	0.56
1:B:362:GLU:HA	1:B:365:ASP:HB2	1.87	0.56
2:C:869:ASN:ND2	2:C:876:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LEU:HD22	1:F:114:ARG:HH11	1.69	0.56
1:R:413:ILE:HG22	2:S:827:TRP:HZ2	1.71	0.56
2:T:813:ALA:HB3	2:T:816:LYS:HB2	1.87	0.55
2:C:804:ILE:O	2:C:826:GLY:HA3	2.06	0.55
2:M:804:ILE:O	2:M:826:GLY:HA3	2.06	0.55
1:B:425:SER:HA	2:C:831:ASN:HD22	1.70	0.55
2:D:863:THR:HG23	2:D:885:THR:HA	1.87	0.55
2:J:813:ALA:HB3	2:J:816:LYS:HB2	1.87	0.55
2:M:839:ARG:NH1	2:M:862:ASP:OD2	2.40	0.55
2:N:826:GLY:O	2:N:844:ARG:NH1	2.37	0.55
2:S:860:PRO:HA	2:S:886:VAL:HG23	1.89	0.55
2:C:839:ARG:NH1	2:C:862:ASP:OD2	2.40	0.55
2:I:841:ILE:HB	2:I:854:GLN:HB3	1.88	0.55
1:B:396:GLN:OE1	2:N:873:ARG:CD	2.55	0.54
2:T:821:VAL:HG11	2:T:853:LEU:HD21	1.89	0.54
1:A:426:GLU:OE1	2:C:808:ARG:NH2	2.40	0.54
2:D:813:ALA:HB3	2:D:816:LYS:HB2	1.90	0.54
1:K:428:ALA:HB2	2:N:831:ASN:HD22	1.73	0.53
1:K:428:ALA:HB2	2:N:831:ASN:ND2	2.23	0.53
1:A:428:ALA:HB2	2:D:831:ASN:ND2	2.24	0.53
2:I:860:PRO:HA	2:I:886:VAL:HG23	1.89	0.53
1:K:426:GLU:OE1	2:M:808:ARG:NH2	2.40	0.53
2:J:821:VAL:HG11	2:J:853:LEU:HD21	1.89	0.53
1:A:428:ALA:HB2	2:D:831:ASN:HD22	1.73	0.53
1:Q:425:SER:HA	2:T:831:ASN:HD22	1.74	0.53
1:L:400:ASP:C	1:L:404:ARG:HH12	2.17	0.52
2:J:824:VAL:HG21	2:J:844:ARG:HG3	1.91	0.52
1:K:434:LEU:HD21	1:L:434:LEU:HB3	1.91	0.52
2:C:862:ASP:O	2:C:866:TYR:OH	2.25	0.52
2:N:813:ALA:HB3	2:N:816:LYS:HB2	1.90	0.52
1:G:425:SER:HA	2:J:831:ASN:HD22	1.74	0.52
2:M:793:LEU:HD12	2:M:855:MET:HE1	1.91	0.52
2:M:842:ILE:HG13	2:M:852:TYR:O	2.09	0.52
2:C:842:ILE:HG13	2:C:852:TYR:O	2.09	0.52
1:A:434:LEU:HD21	1:B:434:LEU:HB3	1.91	0.52
1:B:400:ASP:C	1:B:404:ARG:HH12	2.17	0.52
2:M:823:VAL:HB	2:M:831:ASN:OD1	2.10	0.52
1:L:360:ALA:HA	1:L:363:ARG:HB3	1.92	0.51
2:M:804:ILE:HD12	2:M:844:ARG:HH21	1.75	0.51
1:A:438:ARG:NH1	2:D:817:GLN:HB2	2.23	0.51
2:C:823:VAL:HB	2:C:831:ASN:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:417:GLN:HE21	2:N:827:TRP:HB2	1.75	0.51
2:T:824:VAL:HG21	2:T:844:ARG:HG3	1.91	0.51
1:H:415:GLU:OE1	2:J:805:ASN:ND2	2.43	0.51
2:M:862:ASP:O	2:M:866:TYR:OH	2.26	0.51
1:A:417:GLN:HE21	2:D:827:TRP:HB2	1.75	0.51
2:T:805:ASN:H	2:T:872:TYR:HE1	1.59	0.51
1:B:426:GLU:OE2	2:D:808:ARG:NH1	2.44	0.51
1:R:415:GLU:OE1	2:T:805:ASN:ND2	2.43	0.51
2:C:804:ILE:HD12	2:C:844:ARG:HH21	1.75	0.50
2:M:858:LEU:HD13	2:M:886:VAL:HG11	1.93	0.50
2:J:805:ASN:H	2:J:872:TYR:HE1	1.59	0.50
1:B:360:ALA:HA	1:B:363:ARG:HB3	1.92	0.50
2:I:804:ILE:HG22	2:I:805:ASN:O	2.11	0.50
1:K:438:ARG:NH1	2:N:817:GLN:HB2	2.23	0.50
1:L:426:GLU:OE2	2:N:808:ARG:NH1	2.44	0.50
1:B:409:HIS:O	1:B:413:ILE:HG12	2.12	0.50
2:I:792:ARG:HG2	2:I:854:GLN:HE22	1.77	0.50
2:C:793:LEU:HD12	2:C:855:MET:HE1	1.91	0.50
2:N:832:TYR:CE2	2:N:842:ILE:HG22	2.47	0.50
2:S:792:ARG:HG2	2:S:854:GLN:HE22	1.77	0.50
2:D:832:TYR:CE2	2:D:842:ILE:HG22	2.47	0.50
1:A:416:LEU:HD21	2:C:827:TRP:HH2	1.77	0.49
1:L:409:HIS:O	1:L:413:ILE:HG12	2.12	0.49
2:S:804:ILE:HG22	2:S:805:ASN:O	2.11	0.49
1:B:361:ILE:O	1:B:365:ASP:N	2.43	0.49
2:C:858:LEU:HD13	2:C:886:VAL:HG11	1.93	0.49
1:E:94:LEU:O	1:E:97:ALA:HB3	2.13	0.49
1:K:417:GLN:HE21	2:N:827:TRP:HD1	1.60	0.49
1:O:153:SER:O	1:O:157:VAL:HG23	2.13	0.49
1:E:153:SER:O	1:E:157:VAL:HG23	2.13	0.49
1:E:129:ARG:NH2	1:F:125:SER:OG	2.36	0.49
2:S:832:TYR:O	2:S:837:LYS:NZ	2.34	0.49
1:B:428:ALA:HB2	2:C:831:ASN:ND2	2.28	0.49
1:O:94:LEU:O	1:O:97:ALA:HB3	2.13	0.49
2:D:12:VAL:HG23	2:D:886:VAL:HG23	1.94	0.48
2:I:824:VAL:HG21	2:I:844:ARG:HG3	1.96	0.48
2:S:824:VAL:HG21	2:S:844:ARG:HG3	1.96	0.48
1:O:129:ARG:NH2	1:P:125:SER:OG	2.36	0.48
2:S:826:GLY:O	2:S:844:ARG:NH1	2.46	0.48
2:I:826:GLY:O	2:I:844:ARG:NH1	2.46	0.48
1:K:416:LEU:HD21	2:M:827:TRP:HH2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:832:TYR:HE1	2:C:842:ILE:HG22	1.79	0.48
1:H:441:ARG:CZ	1:K:358:ALA:HB2	2.42	0.48
1:K:367:LEU:HA	1:K:370:SER:HG	1.79	0.48
1:K:391:ARG:NH2	1:L:392:LEU:HD13	2.29	0.48
2:N:12:VAL:HG23	2:N:886:VAL:HG23	1.94	0.48
2:N:863:THR:OG1	2:N:886:VAL:O	2.32	0.48
2:C:832:TYR:CE1	2:C:842:ILE:HG22	2.49	0.47
2:T:824:VAL:HG23	2:T:830:THR:HG22	1.96	0.47
1:L:428:ALA:HB2	2:M:831:ASN:ND2	2.28	0.47
2:M:840:PHE:CD1	2:M:855:MET:HA	2.49	0.47
2:I:855:MET:HE3	2:I:858:LEU:HD11	1.96	0.47
2:J:823:VAL:HG22	2:J:831:ASN:OD1	2.14	0.47
2:N:825:THR:HG22	2:N:826:GLY:H	1.79	0.47
2:M:832:TYR:CE1	2:M:842:ILE:HG22	2.49	0.47
2:T:823:VAL:HG22	2:T:831:ASN:OD1	2.14	0.47
1:E:115:LEU:HD13	1:F:114:ARG:NH1	2.30	0.47
1:A:391:ARG:NH2	1:B:392:LEU:HD13	2.29	0.47
2:D:795:CYS:HB3	2:D:851:VAL:CG1	2.45	0.47
2:D:825:THR:HG22	2:D:826:GLY:H	1.80	0.47
2:D:863:THR:OG1	2:D:886:VAL:O	2.32	0.47
2:J:833:VAL:HG12	2:J:836:VAL:HG22	1.96	0.47
2:C:840:PHE:CD1	2:C:855:MET:HA	2.49	0.47
2:I:832:TYR:O	2:I:837:LYS:NZ	2.34	0.47
1:K:353:VAL:HG13	1:L:357:ARG:HD3	1.97	0.47
1:A:395:MET:HA	1:A:398:ALA:HB3	1.97	0.47
1:H:424:THR:O	2:I:831:ASN:ND2	2.47	0.47
2:N:865:VAL:HG22	2:N:883:GLN:HG3	1.97	0.47
2:M:832:TYR:HE1	2:M:842:ILE:HG22	1.79	0.47
1:Q:405:ASP:O	1:Q:408:THR:OG1	2.31	0.47
2:D:865:VAL:HG22	2:D:883:GLN:HG3	1.97	0.46
2:T:833:VAL:HG12	2:T:836:VAL:HG22	1.96	0.46
2:J:824:VAL:HG23	2:J:830:THR:HG22	1.96	0.46
1:R:424:THR:O	2:S:831:ASN:ND2	2.47	0.46
2:S:855:MET:HE3	2:S:858:LEU:HD11	1.96	0.46
2:T:832:TYR:CE2	2:T:842:ILE:HG22	2.51	0.46
2:I:800:SER:CB	2:I:804:ILE:HG13	2.46	0.46
2:T:863:THR:HA	2:T:884:VAL:O	2.16	0.46
2:N:808:ARG:HG3	2:N:810:TYR:CE1	2.49	0.46
1:O:115:LEU:HB3	1:P:114:ARG:HH12	1.81	0.46
1:O:115:LEU:HD13	1:P:114:ARG:NH1	2.30	0.46
2:T:794:SER:HB3	2:T:850:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:11:LEU:HA	2:N:885:THR:O	2.16	0.46
1:G:425:SER:HA	2:J:831:ASN:ND2	2.31	0.46
1:P:153:SER:O	1:P:157:VAL:HG23	2.16	0.46
1:A:416:LEU:O	1:A:419:THR:OG1	2.32	0.46
1:E:115:LEU:HB3	1:F:114:ARG:HH12	1.81	0.46
1:K:395:MET:HA	1:K:398:ALA:HB3	1.98	0.46
1:L:361:ILE:O	1:L:365:ASP:N	2.44	0.46
2:S:800:SER:CB	2:S:804:ILE:HG13	2.46	0.46
1:A:353:VAL:HG13	1:B:357:ARG:HD3	1.97	0.46
1:F:153:SER:O	1:F:157:VAL:HG23	2.16	0.46
1:Q:425:SER:HA	2:T:831:ASN:ND2	2.31	0.46
2:C:860:PRO:HA	2:C:886:VAL:O	2.16	0.45
2:J:832:TYR:CE2	2:J:842:ILE:HG22	2.51	0.45
2:J:863:THR:HA	2:J:884:VAL:O	2.16	0.45
1:G:405:ASP:O	1:G:408:THR:OG1	2.31	0.45
2:J:794:SER:HB3	2:J:850:THR:HG21	1.98	0.45
2:M:793:LEU:O	2:M:853:LEU:N	2.40	0.45
1:A:417:GLN:HE21	2:D:827:TRP:HD1	1.60	0.45
2:D:824:VAL:HB	2:D:842:ILE:HG13	1.99	0.45
2:M:12:VAL:HG22	2:M:886:VAL:HG12	1.99	0.45
2:D:808:ARG:HG3	2:D:810:TYR:CE1	2.49	0.45
2:N:795:CYS:HB3	2:N:851:VAL:CG1	2.45	0.45
2:M:860:PRO:HA	2:M:886:VAL:O	2.16	0.45
2:M:865:VAL:HG12	2:M:883:GLN:HB2	1.99	0.45
1:B:402:VAL:HA	1:B:405:ASP:HB2	1.99	0.45
1:A:420:ILE:HG23	2:D:806:ILE:HD11	1.99	0.45
1:K:416:LEU:O	1:K:419:THR:OG1	2.31	0.45
2:N:4:LEU:HD23	2:N:797:SER:HA	1.99	0.45
2:T:809:TRP:HZ3	2:T:866:TYR:HB3	1.81	0.45
2:D:799:ARG:HH22	2:D:872:TYR:HB3	1.82	0.45
2:J:809:TRP:HZ3	2:J:866:TYR:HB3	1.81	0.45
2:T:802:ASP:HA	2:T:844:ARG:HH22	1.82	0.45
2:D:11:LEU:HA	2:D:885:THR:O	2.16	0.45
2:C:793:LEU:HD12	2:C:855:MET:CE	2.47	0.45
1:K:434:LEU:HD23	1:L:438:ARG:HH11	1.82	0.45
2:C:2:VAL:HG12	2:C:799:ARG:HG2	1.98	0.45
1:K:420:ILE:HG23	2:N:806:ILE:HD11	1.99	0.44
2:M:2:VAL:HG12	2:M:799:ARG:HG2	1.98	0.44
2:M:793:LEU:HD12	2:M:855:MET:CE	2.47	0.44
2:J:793:LEU:HD12	2:J:853:LEU:HD23	1.99	0.44
2:D:808:ARG:HB3	2:D:823:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:401:GLN:HA	1:L:404:ARG:NH1	2.33	0.44
2:T:2:VAL:HG11	2:T:872:TYR:HD2	1.82	0.44
2:C:865:VAL:HG12	2:C:883:GLN:HB2	1.99	0.44
2:I:831:ASN:C	2:I:831:ASN:OD1	2.60	0.44
2:N:799:ARG:HH22	2:N:872:TYR:HB3	1.82	0.44
2:D:4:LEU:HD23	2:D:797:SER:HA	1.99	0.44
2:J:802:ASP:HA	2:J:844:ARG:HH22	1.82	0.44
1:L:402:VAL:HA	1:L:405:ASP:HB2	1.99	0.44
2:S:831:ASN:OD1	2:S:831:ASN:C	2.60	0.44
2:C:12:VAL:HG22	2:C:886:VAL:HG12	1.99	0.44
2:I:794:SER:HB3	2:I:850:THR:HG21	2.00	0.44
2:T:886:VAL:HG23	2:T:886:VAL:O	2.17	0.44
1:A:434:LEU:HD23	1:B:438:ARG:HH11	1.82	0.44
2:J:2:VAL:HG11	2:J:872:TYR:HD2	1.82	0.44
2:J:886:VAL:HG23	2:J:886:VAL:O	2.17	0.43
2:N:4:LEU:HD22	2:N:795:CYS:SG	2.58	0.43
1:B:401:GLN:HA	1:B:404:ARG:NH1	2.33	0.43
2:D:804:ILE:HA	2:D:872:TYR:CE1	2.53	0.43
2:D:873:ARG:NE	1:L:396:GLN:OE1	2.51	0.43
1:E:97:ALA:HB2	1:F:97:ALA:HB2	2.00	0.43
1:K:353:VAL:HG11	1:L:354:ASP:OD1	2.18	0.43
1:K:367:LEU:HA	1:K:370:SER:OG	2.18	0.43
2:N:824:VAL:HB	2:N:842:ILE:HG13	1.98	0.43
1:Q:404:ARG:HG2	1:Q:405:ASP:N	2.34	0.43
1:A:367:LEU:HA	1:A:370:SER:OG	2.18	0.43
2:D:4:LEU:HD22	2:D:795:CYS:SG	2.58	0.43
1:K:363:ARG:HA	1:K:367:LEU:HD13	2.01	0.43
1:K:378:LEU:HD23	1:K:378:LEU:HA	1.90	0.43
2:N:808:ARG:HB3	2:N:823:VAL:HG22	1.99	0.43
1:O:97:ALA:HB2	1:P:97:ALA:HB2	2.00	0.43
1:Q:431:GLU:OE1	2:T:820:MET:HB2	2.19	0.43
2:T:806:ILE:HA	2:T:824:VAL:O	2.19	0.43
2:C:793:LEU:O	2:C:853:LEU:N	2.40	0.43
1:Q:423:LEU:HD22	1:R:423:LEU:HD23	2.01	0.43
1:A:353:VAL:HG11	1:B:354:ASP:OD1	2.18	0.43
2:S:795:CYS:C	2:S:850:THR:HG23	2.44	0.43
2:I:844:ARG:NH2	2:I:846:SER:OG	2.51	0.43
2:N:804:ILE:HA	2:N:872:TYR:CE1	2.53	0.43
1:O:101:ILE:HA	1:O:104:ILE:HD12	2.01	0.43
2:S:844:ARG:NH2	2:S:846:SER:OG	2.51	0.43
2:J:806:ILE:HA	2:J:824:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:799:ARG:NH2	2:N:872:TYR:HB3	2.34	0.43
2:N:804:ILE:HA	2:N:872:TYR:HE1	1.84	0.43
2:C:832:TYR:HB2	2:C:837:LYS:CG	2.49	0.42
1:G:404:ARG:HG2	1:G:405:ASP:N	2.34	0.42
2:I:842:ILE:HD12	2:I:852:TYR:O	2.19	0.42
2:I:848:LYS:HD3	2:I:852:TYR:OH	2.19	0.42
1:K:417:GLN:HG2	2:N:827:TRP:CD1	2.54	0.42
1:Q:417:GLN:O	1:Q:421:GLU:HG3	2.19	0.42
1:A:356:ALA:HB3	1:B:357:ARG:HD2	2.02	0.42
1:A:363:ARG:HA	1:A:367:LEU:HD13	2.01	0.42
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.90	0.42
1:B:383:GLU:O	1:B:387:GLN:HG2	2.19	0.42
2:M:832:TYR:HB3	2:M:836:VAL:HG23	2.01	0.42
1:P:100:GLN:O	1:P:104:ILE:HG13	2.19	0.42
1:F:100:GLN:O	1:F:104:ILE:HG13	2.19	0.42
1:G:417:GLN:O	1:G:421:GLU:HG3	2.19	0.42
2:I:793:LEU:O	2:I:853:LEU:N	2.52	0.42
2:S:794:SER:HB3	2:S:850:THR:HG21	2.00	0.42
2:T:793:LEU:HD12	2:T:853:LEU:HD23	1.99	0.42
2:T:826:GLY:O	2:T:844:ARG:NH1	2.52	0.42
1:A:417:GLN:HE22	2:D:825:THR:HG22	1.84	0.42
2:D:799:ARG:NH2	2:D:872:TYR:HB3	2.34	0.42
2:D:811:ARG:HB3	2:D:866:TYR:CE2	2.55	0.42
1:G:431:GLU:OE1	2:J:820:MET:HB2	2.19	0.42
2:N:3:GLN:H	2:N:798:SER:HB3	1.84	0.42
2:N:5:GLN:HB3	2:N:796:ALA:HB3	2.02	0.42
2:D:804:ILE:HA	2:D:872:TYR:HE1	1.84	0.42
2:C:832:TYR:HB3	2:C:836:VAL:HG23	2.01	0.42
1:G:423:LEU:HD22	1:H:423:LEU:HD23	2.01	0.42
2:I:795:CYS:C	2:I:850:THR:HG23	2.44	0.42
2:N:807:MET:O	2:N:824:VAL:HG12	2.20	0.42
2:N:808:ARG:NH1	2:N:871:ILE:HD11	2.34	0.42
2:N:811:ARG:HB3	2:N:866:TYR:CE2	2.55	0.42
2:S:842:ILE:HD12	2:S:852:TYR:O	2.19	0.42
1:A:417:GLN:HG2	2:D:827:TRP:CD1	2.55	0.42
1:B:396:GLN:HB3	2:N:873:ARG:CZ	2.50	0.42
1:K:417:GLN:HE22	2:N:825:THR:HG22	1.84	0.42
2:T:825:THR:HG22	2:T:826:GLY:H	1.85	0.42
2:D:808:ARG:NH1	2:D:871:ILE:HD11	2.34	0.42
2:J:826:GLY:O	2:J:844:ARG:NH1	2.52	0.42
2:D:3:GLN:H	2:D:798:SER:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:807:MET:O	2:D:824:VAL:HG12	2.20	0.42
1:G:423:LEU:CD2	1:H:423:LEU:HB3	2.50	0.42
1:L:422:ARG:O	1:L:426:GLU:HG3	2.20	0.42
1:Q:423:LEU:CD2	1:R:423:LEU:HB3	2.50	0.42
1:B:396:GLN:OE1	2:N:873:ARG:NE	2.51	0.42
2:I:6:GLU:HG2	2:I:882:THR:HG23	2.02	0.42
2:J:7:SER:O	2:J:882:THR:HG21	2.19	0.42
2:T:807:MET:O	2:T:824:VAL:HG12	2.20	0.42
2:D:5:GLN:HB3	2:D:796:ALA:HB3	2.02	0.41
2:D:873:ARG:CZ	1:L:396:GLN:HB3	2.49	0.41
1:E:115:LEU:CD1	1:F:111:VAL:HG13	2.49	0.41
1:E:147:ARG:O	1:E:151:LEU:HG	2.20	0.41
1:K:356:ALA:HB3	1:L:357:ARG:HD2	2.02	0.41
2:D:873:ARG:CD	1:L:396:GLN:CD	2.94	0.41
2:N:855:MET:HE1	2:N:866:TYR:CZ	2.55	0.41
2:T:7:SER:O	2:T:882:THR:HG21	2.19	0.41
1:B:422:ARG:O	1:B:426:GLU:HG3	2.20	0.41
1:E:101:ILE:HA	1:E:104:ILE:HD12	2.00	0.41
2:N:825:THR:HG22	2:N:826:GLY:N	2.35	0.41
2:T:842:ILE:HA	2:T:852:TYR:O	2.21	0.41
2:D:855:MET:HE1	2:D:866:TYR:CZ	2.55	0.41
2:J:807:MET:O	2:J:824:VAL:HG12	2.20	0.41
2:S:806:ILE:H	2:S:806:ILE:HG12	1.67	0.41
2:J:825:THR:HG22	2:J:826:GLY:H	1.85	0.41
1:E:127:ALA:O	1:E:131:THR:HG23	2.21	0.41
1:E:139:ASN:HD21	1:F:139:ASN:HB3	1.86	0.41
1:G:433:ALA:HB3	1:H:435:GLU:OE2	2.21	0.41
1:L:383:GLU:O	1:L:387:GLN:HG2	2.19	0.41
2:M:866:TYR:O	2:M:881:GLY:HA2	2.20	0.41
1:O:100:GLN:O	1:P:104:ILE:HD11	2.20	0.41
2:C:866:TYR:O	2:C:881:GLY:HA2	2.20	0.41
2:I:855:MET:HE3	2:I:858:LEU:HD21	2.03	0.41
2:J:789:ASP:HB3	2:J:790:SER:H	1.66	0.41
1:O:139:ASN:HD21	1:P:139:ASN:HB3	1.86	0.41
1:Q:433:ALA:HB3	1:R:435:GLU:OE2	2.21	0.41
2:S:848:LYS:HD3	2:S:852:TYR:OH	2.19	0.41
2:I:825:THR:HG22	2:I:826:GLY:N	2.35	0.41
2:J:793:LEU:HB2	2:J:853:LEU:HB3	2.03	0.41
1:O:127:ALA:O	1:O:131:THR:HG23	2.21	0.41
2:S:855:MET:HE3	2:S:858:LEU:HD21	2.03	0.41
2:D:825:THR:HG22	2:D:826:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:808:ARG:NH1	2:C:876:GLU:OE2	2.54	0.41
2:C:813:ALA:HB3	2:C:816:LYS:HD3	2.03	0.41
1:E:100:GLN:O	1:F:104:ILE:HD11	2.20	0.41
2:J:863:THR:HG23	2:J:885:THR:HA	2.02	0.41
1:Q:406:SER:HA	1:Q:409:HIS:ND1	2.36	0.41
2:S:823:VAL:O	2:S:842:ILE:HG21	2.20	0.41
1:B:417:GLN:O	1:B:421:GLU:HG3	2.21	0.41
2:C:791:LEU:HD12	2:C:791:LEU:HA	1.95	0.41
2:M:808:ARG:NH1	2:M:876:GLU:OE2	2.54	0.41
2:M:811:ARG:HD3	2:M:821:VAL:HG11	2.03	0.41
2:M:2:VAL:HG22	2:M:877:TYR:CD2	2.56	0.40
1:O:147:ARG:O	1:O:151:LEU:HG	2.20	0.40
2:T:793:LEU:HB2	2:T:853:LEU:HB3	2.03	0.40
2:T:863:THR:HG23	2:T:885:THR:HA	2.02	0.40
1:E:139:ASN:HD21	1:F:139:ASN:CB	2.34	0.40
2:S:6:GLU:OE1	2:S:6:GLU:N	2.54	0.40
1:A:417:GLN:NE2	2:D:827:TRP:HB2	2.36	0.40
2:I:811:ARG:HA	2:I:865:VAL:O	2.21	0.40
1:L:417:GLN:O	1:L:421:GLU:HG3	2.21	0.40
2:S:6:GLU:HG2	2:S:882:THR:HG23	2.02	0.40
1:G:406:SER:HA	1:G:409:HIS:ND1	2.36	0.40
2:M:791:LEU:HD12	2:M:791:LEU:HA	1.95	0.40
2:M:813:ALA:HB3	2:M:816:LYS:HD3	2.03	0.40
2:M:825:THR:HG22	2:M:826:GLY:H	1.87	0.40
2:S:825:THR:HG22	2:S:826:GLY:N	2.35	0.40
2:C:811:ARG:HD3	2:C:821:VAL:HG11	2.03	0.40
2:I:6:GLU:N	2:I:6:GLU:OE1	2.54	0.40
2:J:842:ILE:HA	2:J:852:TYR:O	2.21	0.40
1:O:139:ASN:HD21	1:P:139:ASN:CB	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	70/347 (20%)	70 (100%)	0	100	100
1	B	71/347 (20%)	71 (100%)	0	100	100
1	E	61/347 (18%)	61 (100%)	0	100	100
1	F	61/347 (18%)	61 (100%)	0	100	100
1	G	32/347 (9%)	32 (100%)	0	100	100
1	H	28/347 (8%)	28 (100%)	0	100	100
1	K	70/347 (20%)	70 (100%)	0	100	100
1	L	71/347 (20%)	71 (100%)	0	100	100
1	O	61/347 (18%)	61 (100%)	0	100	100
1	P	61/347 (18%)	61 (100%)	0	100	100
1	Q	32/347 (9%)	32 (100%)	0	100	100
1	R	28/347 (8%)	28 (100%)	0	100	100
2	C	94/749 (13%)	94 (100%)	0	100	100
2	D	94/749 (13%)	94 (100%)	0	100	100
2	I	93/749 (12%)	93 (100%)	0	100	100
2	J	94/749 (13%)	94 (100%)	0	100	100
2	M	94/749 (13%)	94 (100%)	0	100	100
2	N	94/749 (13%)	94 (100%)	0	100	100
2	S	93/749 (12%)	93 (100%)	0	100	100
2	T	94/749 (13%)	94 (100%)	0	100	100
All	All	1396/10156 (14%)	1396 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	GLN

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Mol	Chain	Res	Type
1	B	417	GLN
2	D	831	ASN
2	C	5	GLN
1	H	409	HIS
2	I	5	GLN
1	K	399	GLN
1	L	417	GLN
2	N	831	ASN
1	R	409	HIS
2	S	5	GLN
2	T	817	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.

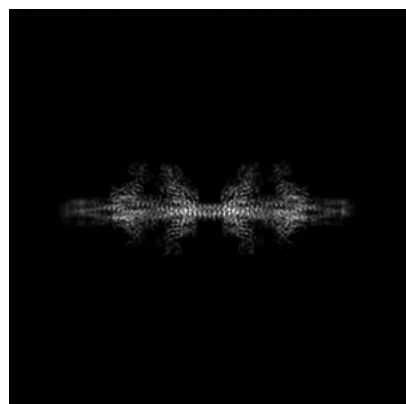
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15398. These allow visual inspection of the internal detail of the map and identification of artifacts.

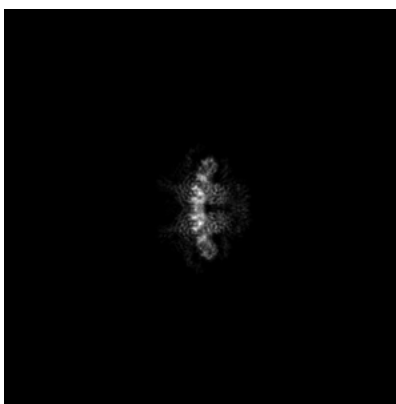
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

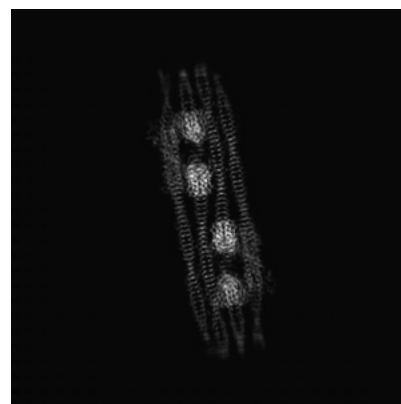
6.1.1 Primary map



X

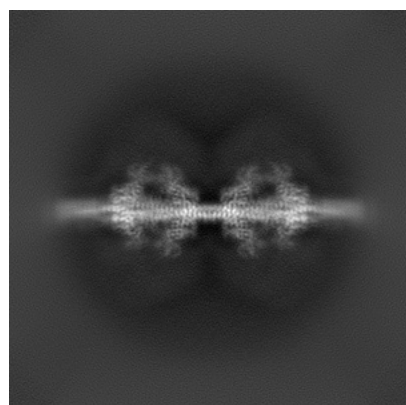


Y

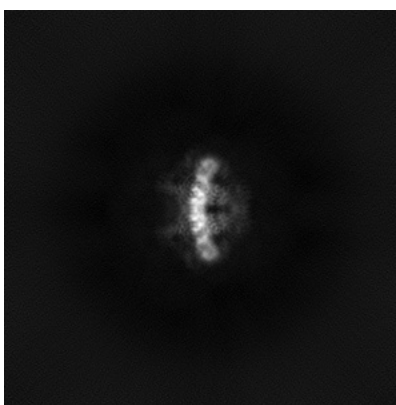


Z

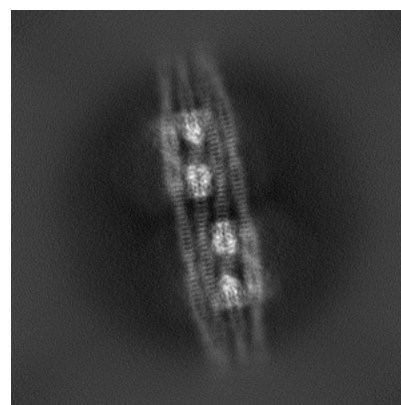
6.1.2 Raw map



X



Y

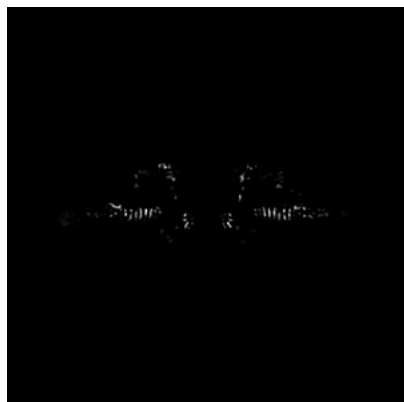


Z

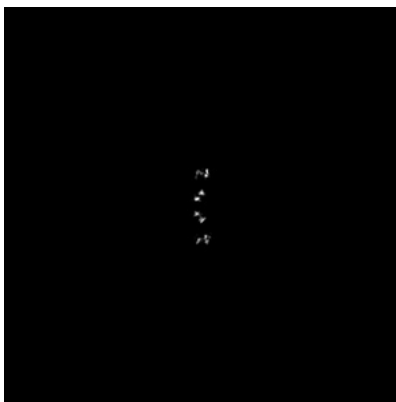
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



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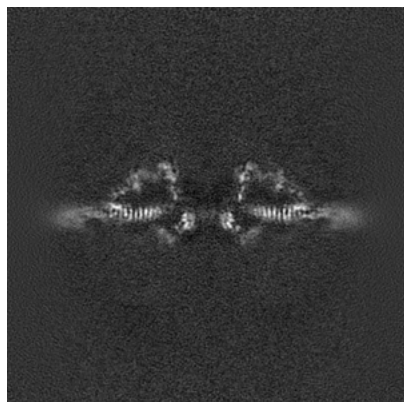


Y Index: 160

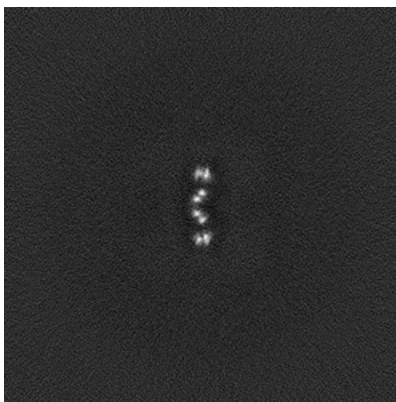


Z Index: 160

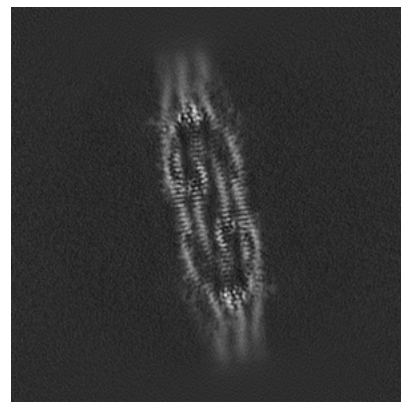
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 172



Y Index: 140

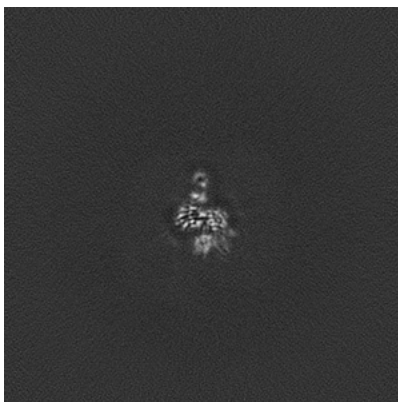


Z Index: 156

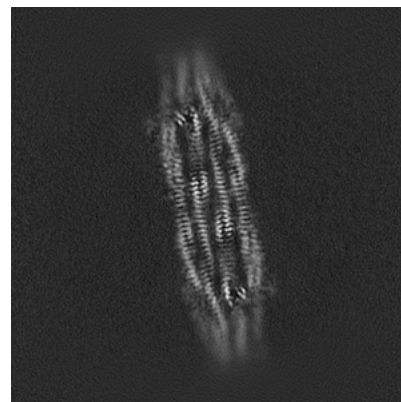
6.3.2 Raw map



X Index: 172



Y Index: 180

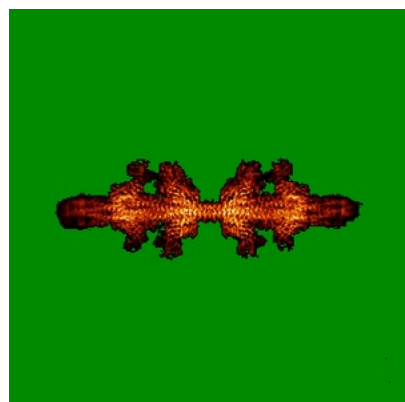


Z Index: 158

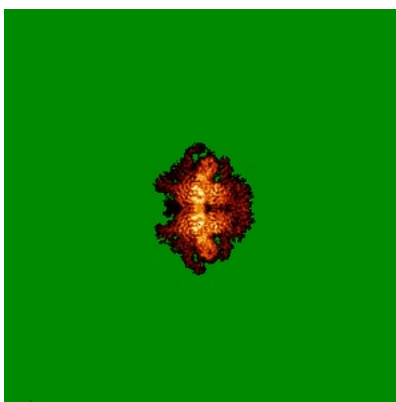
The images above show the largest variance slices of the map in three orthogonal directions.

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

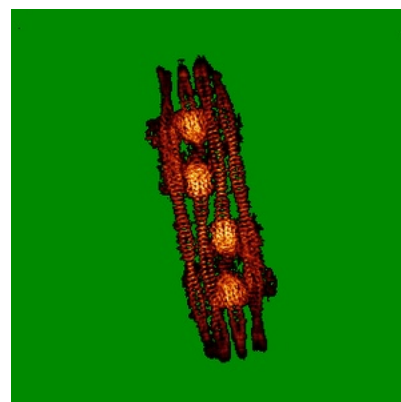
6.4.1 Primary map



X

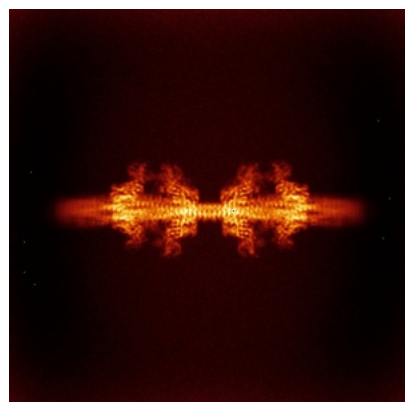


Y

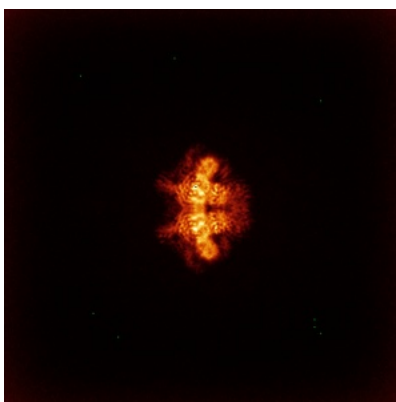


Z

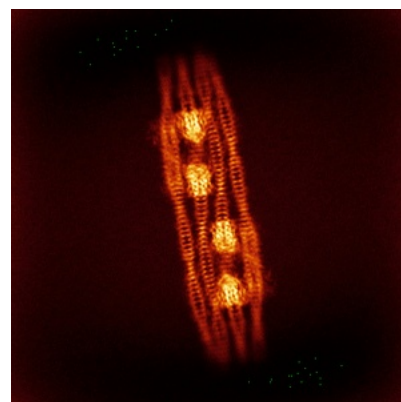
6.4.2 Raw map



X



Y

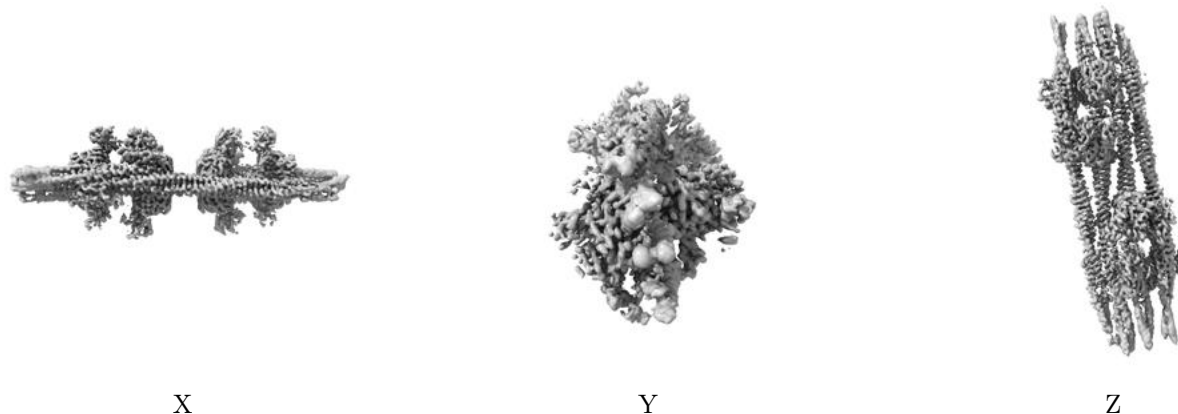


Z

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

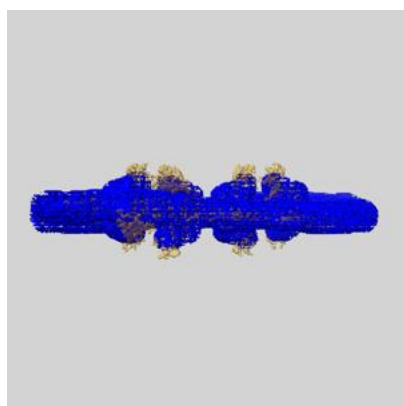
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

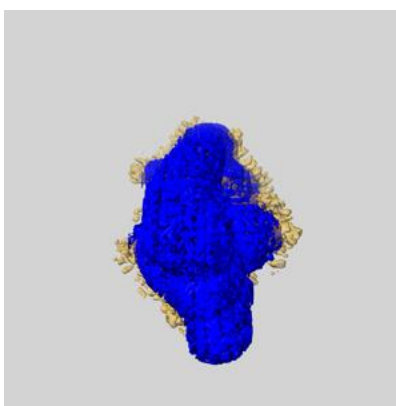
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

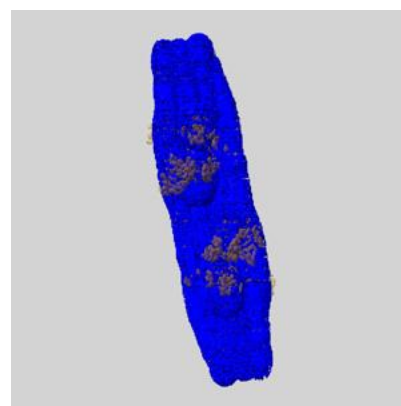
6.6.1 emd_15398_msk_1.map [i](#)



X



Y

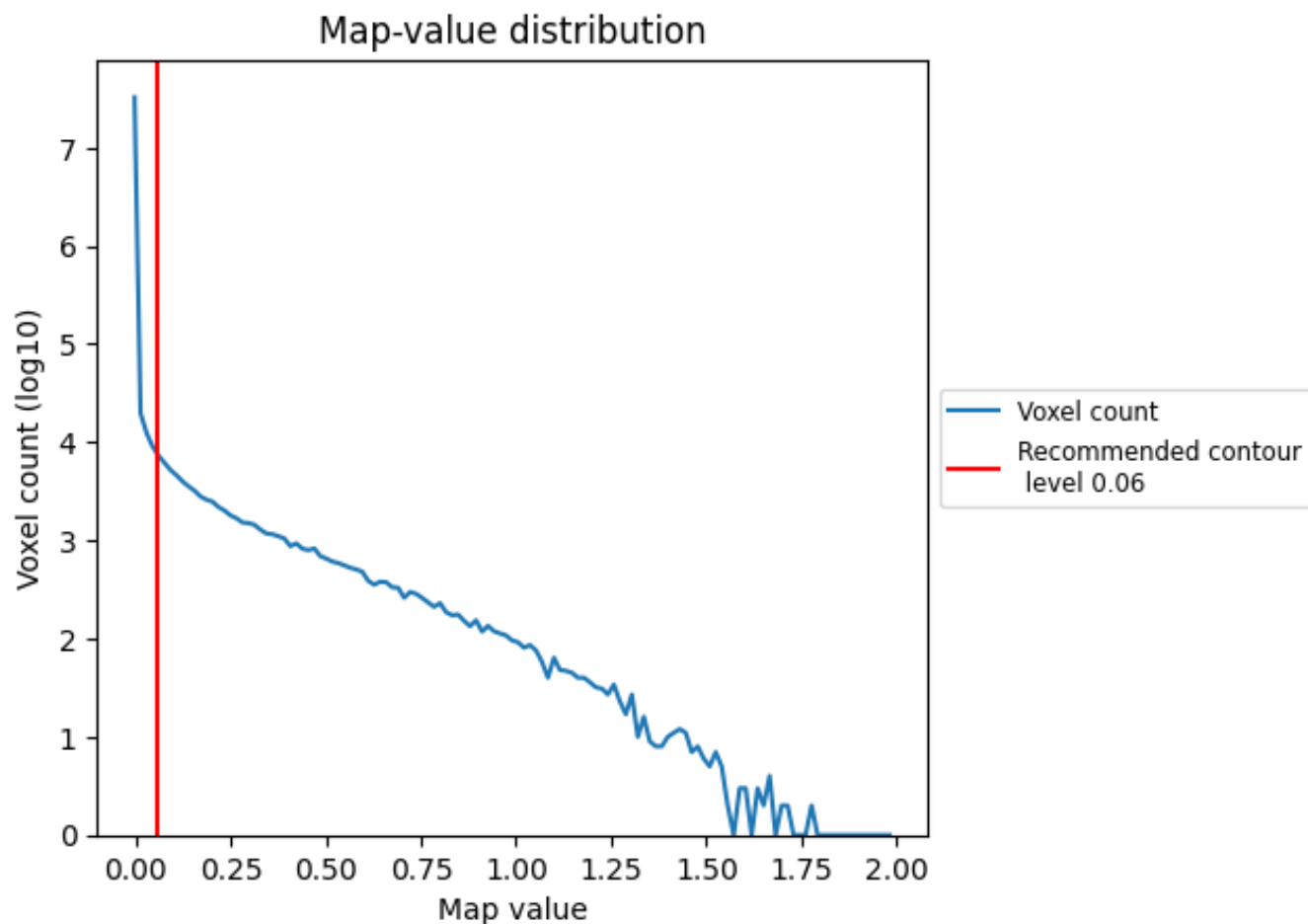


Z

7 Map analysis [i](#)

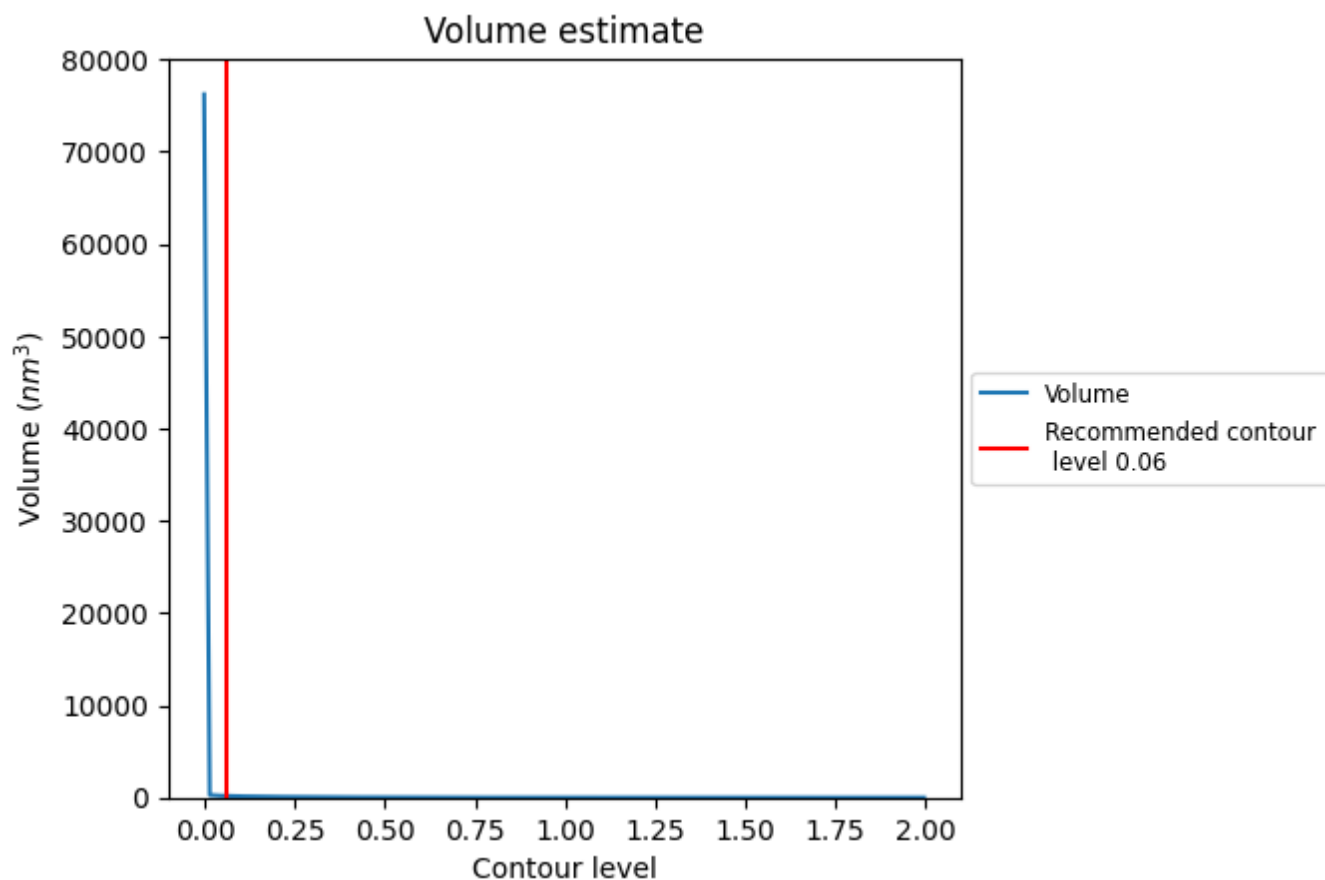
This section contains the results of statistical analysis of the map.

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.

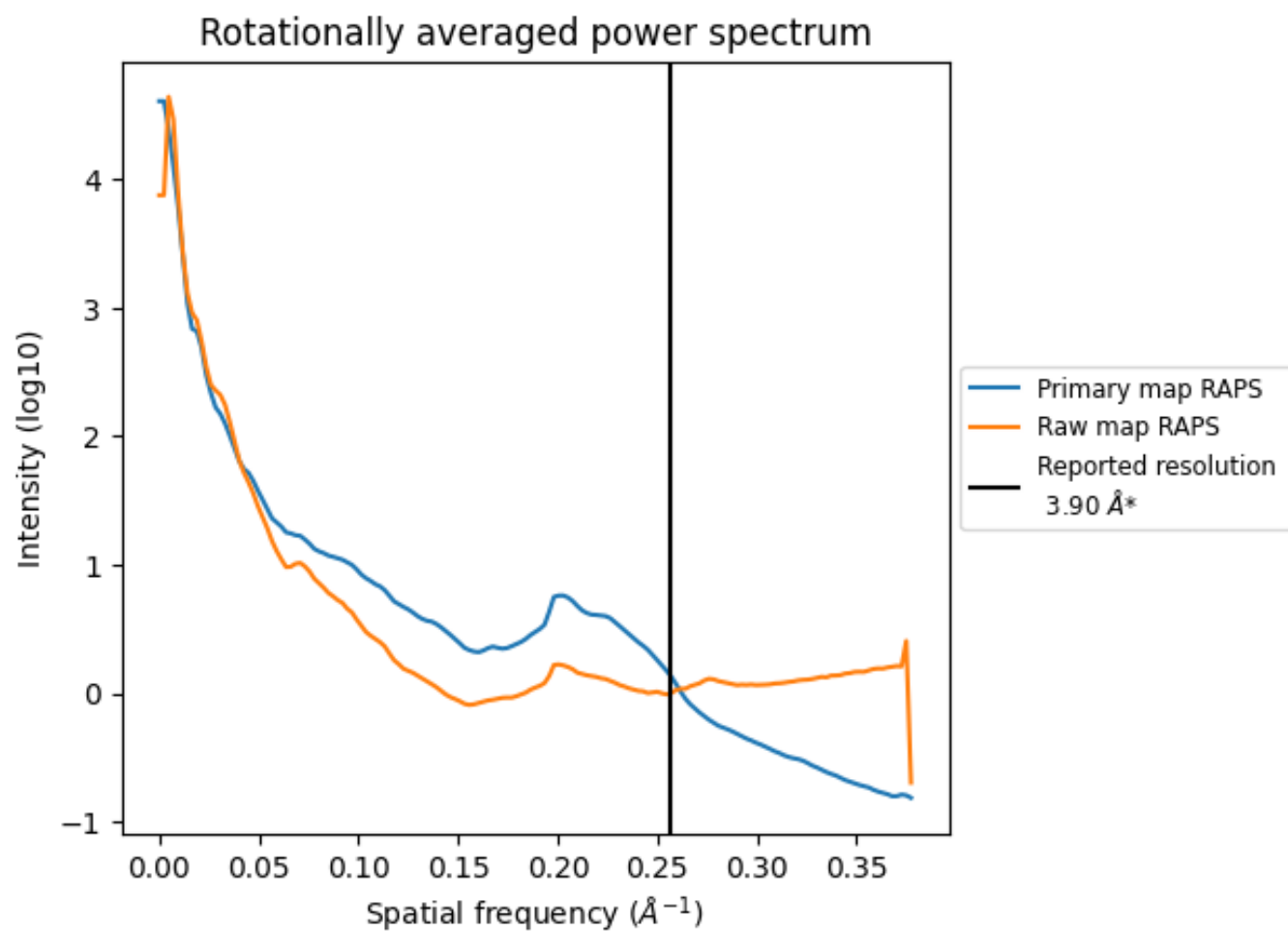
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm^3 ; this corresponds to an approximate mass of 160 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

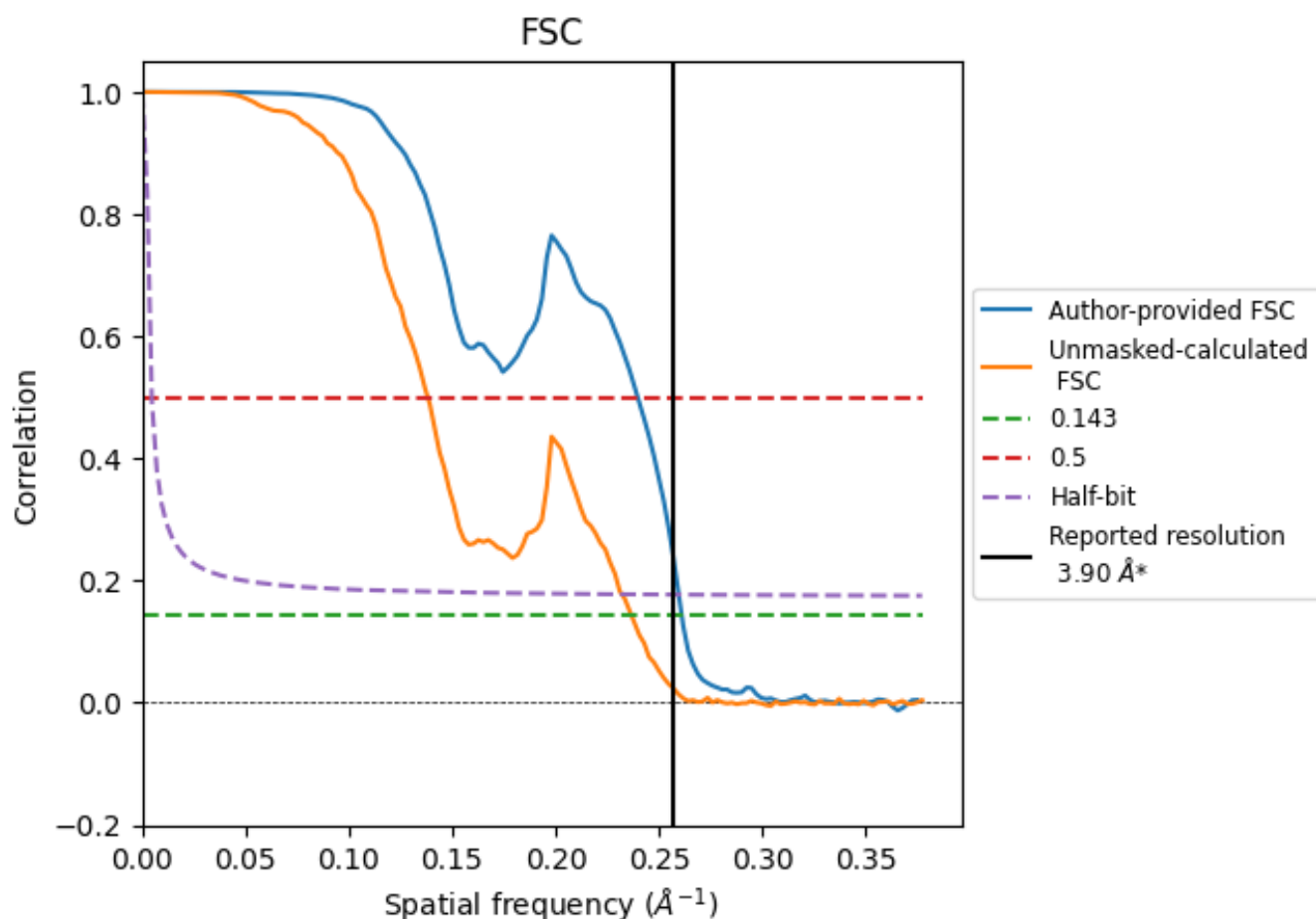


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 $0.256 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

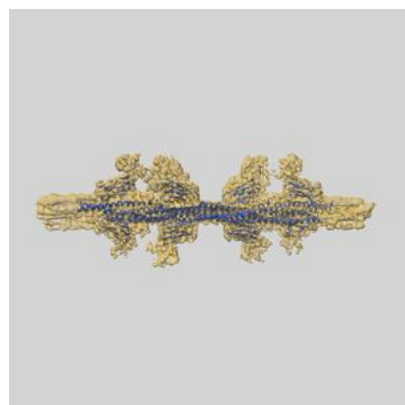
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.83	4.17	3.85
Unmasked-calculated*	4.22	7.24	4.31

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

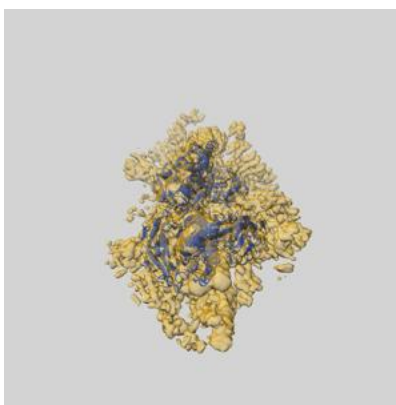
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15398 and PDB model 8AFH. Per-residue inclusion information can be found in section 3 on page 7.

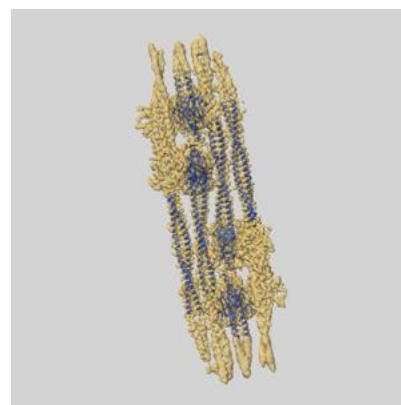
9.1 Map-model overlay [i](#)



X



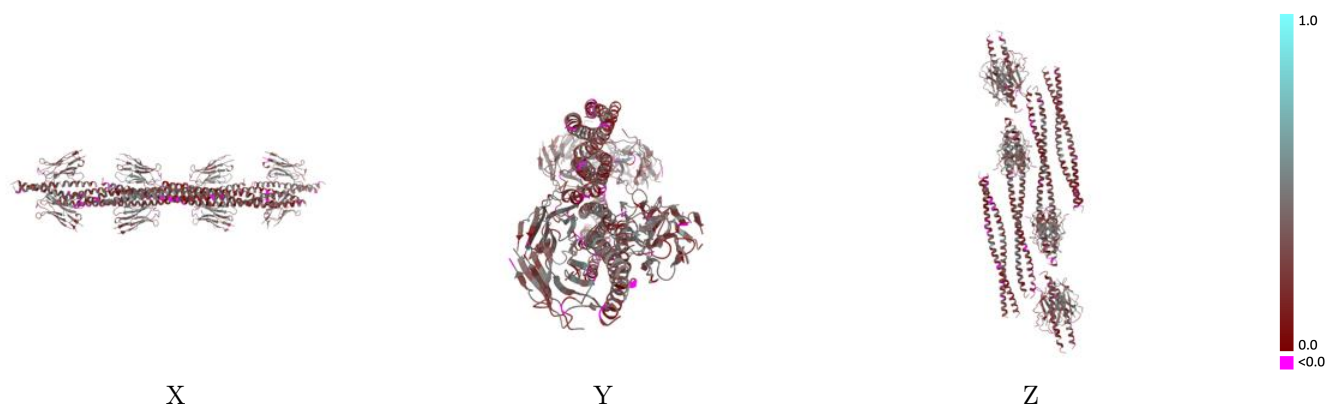
Y



Z

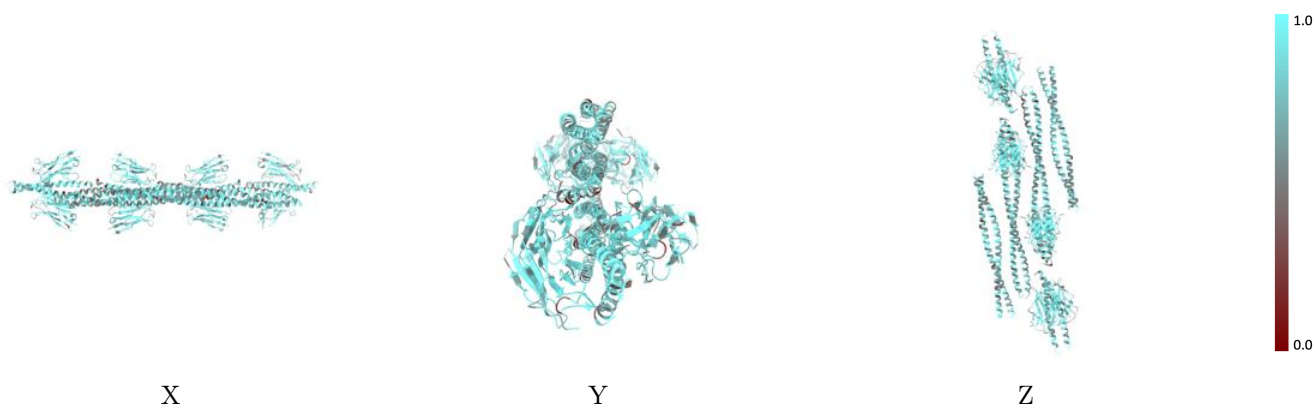
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



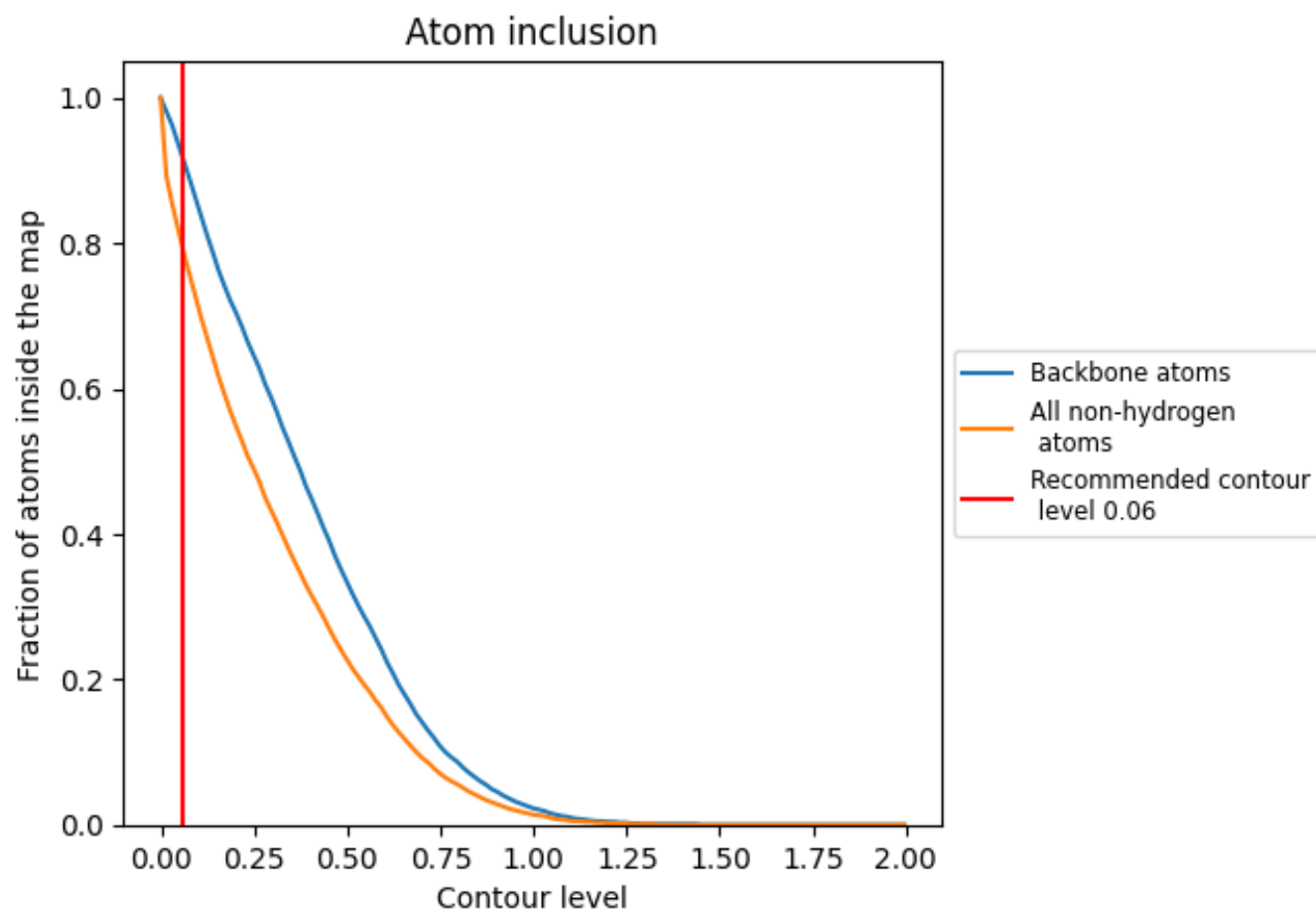
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 79% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.3100
A	 0.7480	 0.2680
B	 0.8040	 0.3270
C	 0.8420	 0.3670
D	 0.8420	 0.3710
E	 0.7120	 0.1900
F	 0.7500	 0.2400
G	 0.7650	 0.3030
H	 0.8330	 0.3240
I	 0.8350	 0.3390
J	 0.7770	 0.3300
K	 0.7180	 0.2710
L	 0.7890	 0.3030
M	 0.8330	 0.3600
N	 0.8100	 0.3550
O	 0.7180	 0.2030
P	 0.7570	 0.2640
Q	 0.7870	 0.2970
R	 0.7840	 0.2810
S	 0.7930	 0.3510
T	 0.7980	 0.3160

