



Full wwPDB EM Validation Report ⓘ

Jul 28, 2026 – 04:51 PM EDT

PDB ID : 9Z5N / pdb_00009z5n
EMDB ID : EMD-73819
Title : Cryo-EM structure of rabbit vault cap
Authors : Li, H.; Clarke, O.B.
Deposited on : 2025-11-12
Resolution : 2.25 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.dev133
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) : 2.50

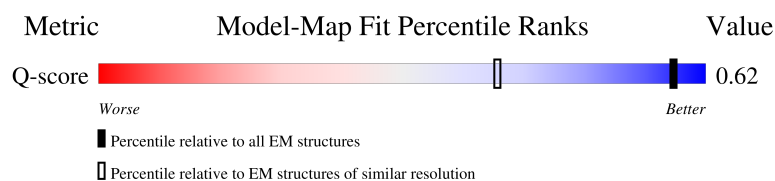
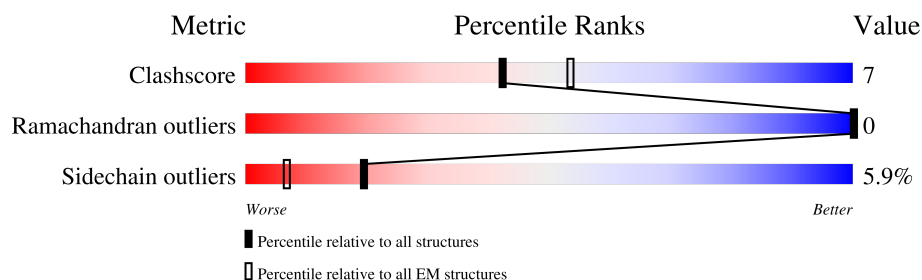
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.25 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	3458 (1.75 - 2.75)

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	140	
1	B	140	
1	C	140	
1	D	140	

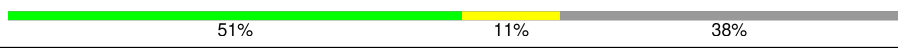
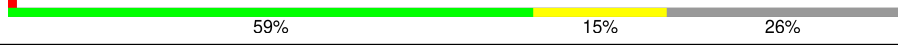
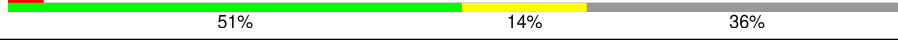
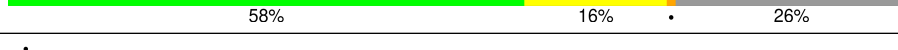
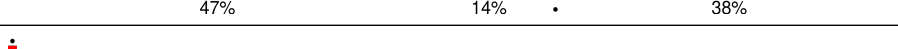
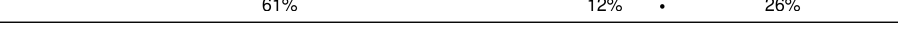
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Mol	Chain	Length	Quality of chain
1	E	140	
1	F	140	
1	G	140	
1	H	140	
1	I	140	
1	J	140	
1	K	140	
1	L	140	
1	M	140	
1	N	140	
1	O	140	
1	P	140	
1	Q	140	
1	R	140	
1	S	140	
1	T	140	
1	U	140	
1	V	140	
1	W	140	
1	X	140	
1	Y	140	
1	Z	140	
1	a	140	
1	b	140	
1	c	140	

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Mol	Chain	Length	Quality of chain
1	d	140	
1	e	140	
1	f	140	
1	g	140	
1	h	140	
1	i	140	
1	j	140	
1	k	140	
1	l	140	
1	m	140	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 56719 atoms, of which 29016 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 vault protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	90	Total	C	H	N	O	S	0	0
			1398	430	715	116	135	2		
1	A	87	Total	C	H	N	O	S	0	0
			1353	424	692	112	123	2		
1	C	104	Total	C	H	N	O	S	0	0
			1612	499	825	132	154	2		
1	D	90	Total	C	H	N	O	S	0	0
			1398	430	715	116	135	2		
1	E	87	Total	C	H	N	O	S	0	0
			1353	424	692	112	123	2		
1	F	104	Total	C	H	N	O	S	0	0
			1612	499	825	132	154	2		
1	G	90	Total	C	H	N	O	S	0	0
			1398	430	715	116	135	2		
1	H	87	Total	C	H	N	O	S	0	0
			1353	424	692	112	123	2		
1	I	104	Total	C	H	N	O	S	0	0
			1612	499	825	132	154	2		
1	J	90	Total	C	H	N	O	S	0	0
			1398	430	715	116	135	2		
1	K	87	Total	C	H	N	O	S	0	0
			1353	424	692	112	123	2		
1	L	104	Total	C	H	N	O	S	0	0
			1612	499	825	132	154	2		
1	M	90	Total	C	H	N	O	S	0	0
			1398	430	715	116	135	2		
1	N	87	Total	C	H	N	O	S	0	0
			1353	424	692	112	123	2		
1	O	104	Total	C	H	N	O	S	0	0
			1612	499	825	132	154	2		
1	P	90	Total	C	H	N	O	S	0	0
			1398	430	715	116	135	2		
1	Q	87	Total	C	H	N	O	S	0	0
			1353	424	692	112	123	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	104	Total 1612	C 499	H 825	N 132	O 154	S 2	0	0
1	S	90	Total 1398	C 430	H 715	N 116	O 135	S 2	0	0
1	T	87	Total 1353	C 424	H 692	N 112	O 123	S 2	0	0
1	U	104	Total 1612	C 499	H 825	N 132	O 154	S 2	0	0
1	V	90	Total 1398	C 430	H 715	N 116	O 135	S 2	0	0
1	W	87	Total 1353	C 424	H 692	N 112	O 123	S 2	0	0
1	X	104	Total 1612	C 499	H 825	N 132	O 154	S 2	0	0
1	Y	90	Total 1398	C 430	H 715	N 116	O 135	S 2	0	0
1	Z	87	Total 1353	C 424	H 692	N 112	O 123	S 2	0	0
1	a	104	Total 1612	C 499	H 825	N 132	O 154	S 2	0	0
1	b	90	Total 1398	C 430	H 715	N 116	O 135	S 2	0	0
1	c	87	Total 1353	C 424	H 692	N 112	O 123	S 2	0	0
1	d	104	Total 1612	C 499	H 825	N 132	O 154	S 2	0	0
1	e	90	Total 1398	C 430	H 715	N 116	O 135	S 2	0	0
1	f	87	Total 1353	C 424	H 692	N 112	O 123	S 2	0	0
1	g	104	Total 1612	C 499	H 825	N 132	O 154	S 2	0	0
1	h	90	Total 1398	C 430	H 715	N 116	O 135	S 2	0	0
1	i	87	Total 1353	C 424	H 692	N 112	O 123	S 2	0	0
1	j	104	Total 1612	C 499	H 825	N 132	O 154	S 2	0	0
1	k	90	Total 1398	C 430	H 715	N 116	O 135	S 2	0	0
1	l	87	Total 1353	C 424	H 692	N 112	O 123	S 2	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	m	104	Total	C	H	N	O	S	0	0
			1612	499	825	132	154	2		

GLY ARG
PRO MET
THR ILE
ALA THR
GLY GLY
PRO ARG
LEU LEU
GLN GLN
GLU GLU
ALA ALA
ALA ALA
SER SER
PRO PRO
GLN GLN
SER SER
PRO PRO
SER SER
ALA ALA
PRO PRO
LEU LEU
ALA ALA
PRO PRO
GLY GLY
SER SER
THR THR
HIS HIS
ILE ILE
LEU LEU
PRO PRO

• Molecule 1: Major vault protein

Chain E: 51% 10% 38%

LEU ALA
ILE ILE
GLU GLU
T755
R761
V762
Q763
K764
V765
R766
L779
K794
F795
K796
S805
K808
D809
L810
Q818
L822
Q823
S824
K828
SER
THR
LEU
ILE
THR
ASP
GLY
SER
THR
PRO
V839
F846
L851
GLY
ALA
ASP
GLY
GLN
PRO
LEU
GLY
ARG
MET
THR
GLY

GLY PRO
ARG ARG
LEU LEU
GLN GLN
ALA ALA
SER SER
PRO PRO
GLN GLN
SER SER
PRO PRO
SER SER
ALA ALA
PRO PRO
LEU LEU
ALA ALA
PRO PRO
GLY GLY
SER SER
HIS HIS
ILE ILE
LEU LEU
PRO PRO

• Molecule 1: Major vault protein

Chain F: 61% 11% 26%

LEU ALA
ILE ILE
GLU GLU
T755
L759
V762
Q763
E769
Q785
E789
V790
E791
M798
L802
L810
V811
V812
E816
L821
L822
L825
L831
N843
T844
A845
L849
L858
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA
SER
PRO
GLN
SER

PRO SER
SER PRO
PRO PRO
LEU LEU
ALA ALA
PRO PRO
GLY GLY
SER SER
THR THR
HIS HIS
ILE ILE
LEU LEU
PRO PRO

• Molecule 1: Major vault protein

Chain G: 48% 16% 36%

LEU ALA
ILE ILE
GLU GLU
T755
L759
V762
Q763
K764
V765
R766
E767
L768
E769
V770
L771
E778
E791
K794
V795
K796
Q797
M798
V819
L822
L827
K828
G835
S836
T837
P838
V839
N840
L841
F842
N843
T844
ALA
PHE
GLY
LEU
LEU
GLY
GLY
LEU
GLY
ALA
ASP
GLY
GLN
PRO
LEU

GLY ARG
MET MET
THR THR
ALA ALA
GLY GLY
PRO PRO
ARG ARG
LEU LEU
GLN GLN
GLU GLU
ALA ALA
ALA ALA
SER SER
PRO PRO
GLN GLN
SER SER
PRO PRO
SER SER
ALA ALA
PRO PRO
LEU LEU
PRO PRO
GLY GLY
SER SER
THR THR
HIS HIS
ILE ILE
LEU LEU
PRO PRO

• Molecule 1: Major vault protein

Chain H: 50% 11% 38%

LEU ALA
ILE ILE
GLU GLU
T755
R761
V762
Q763
K764
V765
R766
K794
F795
K796
S805
T806
I807
K808
D809
L810
A811
V812
Q818
L822
Q823
S824
K828
SER
THR
LEU
ILE
THR
ASP
GLY
SER
THR
PRO
V839
N840
F846
L851
GLY
ALA
ASP
GLY
GLN
PRO
LEU
GLY
ARG
MET
THR

ALA GLY
GLY GLY
PRO PRO
ARG ARG
LEU LEU
GLN GLN
GLU GLU
ALA ALA
SER SER
PRO PRO
GLN GLN
SER SER
PRO PRO
SER SER
ALA ALA
PRO PRO
LEU LEU
ALA ALA
PRO PRO
GLY GLY
SER SER
THR THR
HIS HIS
ILE ILE
LEU LEU
PRO PRO

• Molecule 1: Major vault protein

Chain I: 59% 14% 26%

LEU ALA
ILE ILE
GLU GLU
T755
E756
A757
E758
L759
V762
R766
E769
L779
E791
L802
I807
L810
A811
V812
E816
L821
L822
L825
L831
F842
N843
T844
A845
A853
L858
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA
SER

PRO
GLN
SER
PRO
SER
ALA
PRO
LEU
ALA
PRO
GLY
THR
HIS
ILE
LEU
PRO

• Molecule 1: Major vault protein

Chain J:



LEU
ALA
ILE
GLU
T755
E756
L759
Q760
R761
V762
Q763
K764
V765
E767
L768
A773
E791
K796
Q797
M798
M817
L822
L827
K828
G835
S836
T837
P838
V839
N840
L841
F842
N843
T844
ALA
PHE
GLY
LEU
LEU
GLY
LEU
GLY
ASP
ALA
GLY
GLN
PRO
GLY
LEU
ARG
MET

THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA
SER
PRO
GLN
SER
SER
SER
ALA
PRO
LEU
ALA
PRO
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THR
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LEU
LEU
PRO

• Molecule 1: Major vault protein

Chain K:



LEU
ALA
ILE
GLU
T755
V762
Q763
K764
V765
R766
E767
L768
L779
K794
F795
K796
S805
K808
D809
L810
A811
P815
E816
M817
Q818
V819
L822
K828
SER
THR
LEU
ILE
THR
ASP
GLY
SER
THR
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V839
L851
GLY
ALA
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LEU
GLY
MET
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LEU
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ALA
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LEU
ALA
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LEU
PRO

• Molecule 1: Major vault protein

Chain L:



LEU
ALA
ILE
GLU
T755
L759
V762
R761
V762
R766
E767
L768
E769
Y772
L779
Q785
E789
V790
E791
K794
M798
L810
A811
L821
L825
L831
F842
N843
L858
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLY
GLN
PRO
LEU
ALA
ALA
SER
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• Molecule 1: Major vault protein

Chain M:



LEU
ALA
ILE
GLU
E756
L759
Q760
R761
V762
R766
E767
L768
L770
E791
K796
Q797
M798
M817
L822
L827
G835
S836
T837
P838
V839
N840
L841
F842
N843
T844
ALA
PHE
GLY
GLY
LEU
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LEU
GLU
ALA
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• Molecule 1: Major vault protein

Chain N:



LEU
ALA
ILE
GLU
T755
L759
Q760
R761
V762
Q763
K764
V765
E767
E791
K794
F795
K796
L810
A811
M817
Q818
L822
Q823
S824
K828
SER
THR
LEU
ILE
THR
ASP
GLY
SER
THR
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V839
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ARG
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GLU
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ALA
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SER
SER
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LEU
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• Molecule 1: Major vault protein

Chain O:  58% 16% 26%

LEU
ALA
ILE
GLU
T755
L759
V762
L768
E769
L779
Q785
E789
V790
E791
M798
L802
L810
A811
V812
E816
M817
L821
L825
G826
L827
K828
L831
F842
N843
L849
A853
L858
GLY
ARG
MET
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GLY
GLY
PRO
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LEU
GLN

GLU
ALA
ALA
SER
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SER
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LEU
ALA
PRO
GLY
SER
THR
HIS
ILE
LEU
PRO

• Molecule 1: Major vault protein

Chain P:  53% 11% 36%

LEU
ALA
ILE
GLU
T755
L759
K764
E791
K794
F795
Q797
M798
N817
Q818
V819
L822
L827
K828
G835
S836
T837
P838
V839
N840
L841
F842
N843
T844
ALA
PHE
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GLY
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GLY
GLY
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• Molecule 1: Major vault protein

Chain Q:  50% 11% 38%

LEU
ALA
ILE
GLU
T755
L759
Q760
R761
V762
K764
V765
R766
K793
K794
F795
K796
K808
V812
M817
Q818
L821
L822
Q823
S824
K828
SER
THR
LEU
ILE
THR
ASP
GLY
SER
THR
PRO
V839
F846
L851
GLY
ALA
ASP
GLY
GLN
GLY
PRO
GLY
LEU
ARG
MET
THR
ALA

GLY
GLY
PRO
PRO
ARG
LEU
GLN
GLU
ALA
ALA
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PRO
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ALA
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PRO

• Molecule 1: Major vault protein

Chain R:  62% 11% 26%

LEU
ALA
GLU
T755
E758
L759
V762
L768
E769
Y772
L779
Q785
E789
V790
E791
K794
M798
L821
L825
L831
N843
A853
L858
GLY
ARG
MET
THR
ALA
GLY
LEU
GLY
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ALA
GLY
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PRO

• Molecule 1: Major vault protein

Chain S:  53% 11% 36%

LEU
ALA
ILE
GLU
T755
L759
V762
V765
E769
A773
E791
K794
F795
Q797
M798
L822
L827
K828
G835
S836
T837
P838
V839
N840
L841
F842
N843
T844
ALA
PHE
GLY
LEU
GLY
LEU
GLY
GLY
ALA
ASP
GLY
GLN
GLY
PRO
LEU
SER
PRO
GLY
ARG
MET
THR
ALA
GLY

PRO ARG
LEU ILE
GLN GLU
ALA ALA
SER SER
PRO PRO
GLN SER
PRO PRO
SER SER
ALA ALA
PRO PRO
LEU LEU
ALA ALA
GLY GLY
SER SER
THR THR
HIS HIS
ILE ILE
LEU LEU
PRO PRO

• Molecule 1: Major vault protein

Chain T: 49% 13% 38%

LEU ALA
ILE ILE
GLU GLU
T755
L759
Q760
R761
V762
V765
R766
E767
L768
L779
K794
F795
Q797
M798
S805
K808
D809
L810
Q818
L821
L822
Q823
S824
L827
K828
SER
THR
LEU
LEU
ILE
THR
ASP
GLY
SER
SER
THR
PRO
V839
F846
L851
GLY
ALA
ASP
GLY
GLN
PRO

LEU
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
SER
PRO
GLN
SER
PRO
SER
SER
ALA
PRO
LEU
ALA
PRO
GLY
SER
THR
HIS
ILE
LEU
PRO

• Molecule 1: Major vault protein

Chain U: 59% 15% 26%

LEU
ALA
ILE
GLU
T755
E756
A757
E758
L759
V762
R766
E767
L768
Y772
L779
K783
E791
A792
K793
K794
Q797
M798
L802
I807
L810
L821
L825
L831
N843
L858
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
SER

PRO
GLN
SER
PRO
ALA
SER
PRO
LEU
PRO
PRO
SER
THR
HIS
ILE
LEU
PRO

• Molecule 1: Major vault protein

Chain V: 48% 16% 36%

LEU
ALA
ILE
GLU
T755
L759
V762
Q763
K764
V765
R766
E767
L768
E769
V771
V772
A773
E778
E791
K796
Q797
M798
M817
L822
L827
K828
G835
S836
T837
P838
V839
N840
L841
F842
N843
T844
ALA
PHE
GLY
LEU
LEU
GLY
LEU
GLY
GLY
ALA
ASP
GLY
GLN
PRO
LEU

GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA
PRO
PRO
SER
SER
ALA
PRO
LEU
PRO
ALA
PRO
GLY
SER
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LEU
PRO

• Molecule 1: Major vault protein

Chain W: 49% 11% 38%

LEU
ALA
ILE
GLU
T755
L759
V762
Q763
K764
V765
R766
Y772
L777
E778
L779
K794
F795
K796
S805
K808
D809
L810
A811
M817
Q818
L821
L822
K828
SER
THR
LEU
ILE
THR
ASP
GLY
SER
SER
PRO
V839
F846
L851
GLY
ALA
ASP
GLY
GLN
PRO
LEU

GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA
PRO
PRO
SER
SER
ALA
PRO
LEU
PRO
ALA
PRO
GLY
SER
THR
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ILE
LEU
PRO

• Molecule 1: Major vault protein

Chain X: 61% 11% 26%

LEU
ALA
ILE
GLU
E756
L759
V765
L768
E769
Y772
K783
A784
Q785
E789
V790
E791
M798
V812
E816
L821
L825
L831
N843
A853
L858
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA
SER
PRO
PRO
GLN
SER
PRO
LEU

LEU	ALA	ILE	GLU	V755	L759	V762	R766	Y772	K793	K794	F795	K796	K808	D809	L810	A811	V812	Q818	L821	L822	G823	S824	K828	SER	THR	LEU	THR	ILE	THR	ASP	GLY	PRO	THR	THR	V839	P840	F846	L851	GLY	ALA	ASP	GLY	GLN	GLN	LEU	LEU	GLY	GLY	ARG	MET	THR
-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA
SER
PRO
GLN
SER
PRO
SER
PRO
GLY
THR
HIS
ILE
LEU
PRO

• Molecule 1: Major vault protein

Chain d: 59% 14% 26%

LEU
ALA
ILE
GLU
T755
E758
L759
V762
L768
E769
L779
K783
E791
K794
M798
L802
I807
L810
A811
V812
E816
K820
L821
L825
L831
N843
A853
L858
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLU
ALA
ALA

• Molecule 1: Major vault protein

Chain e: 53% 10% 36%

LEU
ALA
ILE
GLU
E756
L759
Q760
R761
V762
R766
A773
E791
K796
Q797
M798
L822
L827
K828
G835
S836
T837
P838
V839
N840
L841
P842
N843
T844
ALA
PHE
GLY
LEU
GLY
LEU
GLY
GLY
ASP
GLY
GLN
PRO
LEU
GLY
ARG
MET
THR
ALA
GLY
PRO
ARG

• Molecule 1: Major vault protein

Chain f: 51% 11% 38%

LEU
ALA
ILE
GLU
E756
L759
Q760
R761
V762
Q763
K764
V765
R766
L777
E778
L779
K794
F795
K796
K808
M817
Q818
L822
K828
SER
THR
LEU
ILE
THR
ASP
GLY
SER
THR
PRO
V839
N840
F846
L851
GLY
ALA
ASP
GLY
GLN
PRO
GLY
PRO
LEU
GLY
ARG
MET
THR
ALA

• Molecule 1: Major vault protein

Chain g: 59% 15% 26%

LEU
ALA
ILE
GLU
E755
E756
A757
E758
L759
V762
V765
E769
Y772
L779
K783
E791
K794
M798
A811
V812
E816
M817
L821
L825
L831
N843
A853
L858
GLY
ARG
MET
THR
ALA
GLY
GLY
PRO
ARG
LEU
GLN
GLY
ALA
SER

• Molecule 1: Major vault protein

Chain h: 51% 14% 36%

LEU
ALA
ILE
GLU
T755
L759
V762
Q763
K764
L768
E778
E791
A792
K793
K796
Q797
M798
M817
L822
L827
K828
G835
S836
T837
P838
V839
N840
L841
F842
N843
T844
ALA
PHE
GLY
LEU
LEU
GLY
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129638	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.578	Depositor
Minimum map value	-0.322	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0615	Depositor
Map size (Å)	311.04, 311.04, 311.04	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/665	0.42	0/893
1	B	0.20	0/687	0.33	0/926
1	C	0.22	0/794	0.38	0/1071
1	D	0.20	0/687	0.34	0/926
1	E	0.19	0/665	0.42	0/893
1	F	0.22	0/794	0.39	0/1071
1	G	0.21	0/687	0.36	0/926
1	H	0.19	0/665	0.44	0/893
1	I	0.22	0/794	0.39	0/1071
1	J	0.20	0/687	0.34	0/926
1	K	0.19	0/665	0.43	0/893
1	L	0.21	0/794	0.37	0/1071
1	M	0.20	0/687	0.34	0/926
1	N	0.20	0/665	0.45	0/893
1	O	0.22	0/794	0.40	0/1071
1	P	0.20	0/687	0.34	0/926
1	Q	0.19	0/665	0.44	0/893
1	R	0.22	0/794	0.39	0/1071
1	S	0.20	0/687	0.35	0/926
1	T	0.20	0/665	0.43	0/893
1	U	0.22	0/794	0.38	0/1071
1	V	0.20	0/687	0.35	0/926
1	W	0.19	0/665	0.42	0/893
1	X	0.22	0/794	0.41	0/1071
1	Y	0.20	0/687	0.34	0/926
1	Z	0.19	0/665	0.43	0/893
1	a	0.22	0/794	0.40	0/1071
1	b	0.20	0/687	0.34	0/926
1	c	0.19	0/665	0.43	0/893
1	d	0.22	0/794	0.38	0/1071
1	e	0.20	0/687	0.33	0/926
1	f	0.19	0/665	0.42	0/893
1	g	0.22	0/794	0.41	0/1071
1	h	0.20	0/687	0.34	0/926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.19	0/665	0.43	0/893
1	j	0.22	0/794	0.38	0/1071
1	k	0.20	0/687	0.33	0/926
1	l	0.19	0/665	0.44	0/893
1	m	0.22	0/794	0.38	0/1071
All	All	0.21	0/27898	0.39	0/37570

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	661	692	692	10	0
1	B	683	715	715	17	0
1	C	787	825	825	17	0
1	D	683	715	715	17	0
1	E	661	692	692	9	0
1	F	787	825	825	18	0
1	G	683	715	715	20	0
1	H	661	692	692	11	0
1	I	787	825	825	19	0
1	J	683	715	715	18	0
1	K	661	692	692	12	0
1	L	787	825	825	16	0
1	M	683	715	715	14	0
1	N	661	692	692	10	0
1	O	787	825	825	21	0
1	P	683	715	715	16	0
1	Q	661	692	692	11	0
1	R	787	825	825	16	0
1	S	683	715	715	17	0
1	T	661	692	692	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	787	825	825	18	0
1	V	683	715	715	18	0
1	W	661	692	692	14	0
1	X	787	825	825	15	0
1	Y	683	715	715	18	0
1	Z	661	692	692	12	0
1	a	787	825	825	14	0
1	b	683	715	715	18	0
1	c	661	692	692	10	0
1	d	787	825	825	21	0
1	e	683	715	715	16	0
1	f	661	692	692	12	0
1	g	787	825	825	14	0
1	h	683	715	715	17	0
1	i	661	692	692	11	0
1	j	787	825	825	20	0
1	k	683	715	715	19	0
1	l	661	692	692	18	0
1	m	787	825	825	16	0
All	All	27703	29016	29016	381	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 7.

All (381) 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:d:798:MET:HE1	1:f:846:PHE:CZ	2.19	0.78
1:S:769:GLU:OE2	1:U:766:ARG:NH2	2.20	0.75
1:B:841:LEU:HD12	1:D:839:VAL:HG13	1.69	0.73
1:P:841:LEU:HD12	1:S:839:VAL:HG13	1.69	0.73
1:F:769:GLU:OE1	1:H:766:ARG:NH2	2.22	0.73
1:j:798:MET:HE1	1:l:846:PHE:CZ	2.23	0.73
1:D:841:LEU:HD12	1:G:839:VAL:HG13	1.71	0.72
1:R:798:MET:HE1	1:T:846:PHE:HZ	1.54	0.72
1:Y:827:LEU:HD21	1:a:831:LEU:HB2	1.71	0.72
1:R:798:MET:HE1	1:T:846:PHE:CZ	2.24	0.72
1:k:827:LEU:HD21	1:m:831:LEU:HB2	1.72	0.72
1:b:827:LEU:HD21	1:d:831:LEU:HB2	1.72	0.71
1:D:827:LEU:HD21	1:F:831:LEU:HB2	1.73	0.71
1:F:825:LEU:HD21	1:G:822:LEU:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:827:LEU:HD21	1:g:831:LEU:HB2	1.73	0.71
1:G:827:LEU:HD21	1:I:831:LEU:HB2	1.72	0.71
1:h:827:LEU:HD21	1:j:831:LEU:HB2	1.73	0.71
1:B:827:LEU:HD21	1:C:831:LEU:HB2	1.73	0.70
1:l:761:ARG:O	1:l:765:VAL:HG23	1.90	0.70
1:O:769:GLU:OE1	1:Q:766:ARG:NH2	2.25	0.70
1:J:827:LEU:HD21	1:L:831:LEU:HB2	1.72	0.70
1:S:827:LEU:HD21	1:U:831:LEU:HB2	1.73	0.70
1:P:827:LEU:HD21	1:R:831:LEU:HB2	1.72	0.70
1:M:827:LEU:HD21	1:O:831:LEU:HB2	1.72	0.70
1:J:791:GLU:OE1	1:K:794:LYS:NZ	2.26	0.69
1:V:827:LEU:HD21	1:X:831:LEU:HB2	1.74	0.69
1:M:759:LEU:HD21	1:N:764:LYS:HB3	1.74	0.69
1:k:791:GLU:OE1	1:l:794:LYS:NZ	2.26	0.68
1:I:769:GLU:OE1	1:K:766:ARG:NH1	2.27	0.68
1:S:759:LEU:HD13	1:T:768:LEU:HD12	1.75	0.67
1:d:798:MET:HE1	1:f:846:PHE:HZ	1.58	0.67
1:F:821:LEU:HD23	1:F:849:LEU:HD22	1.77	0.66
1:V:841:LEU:HD12	1:Y:839:VAL:HG13	1.77	0.66
1:b:764:LYS:HB3	1:d:759:LEU:HD11	1.78	0.65
1:E:761:ARG:O	1:E:765:VAL:HG23	1.96	0.65
1:O:821:LEU:HD23	1:O:849:LEU:HD22	1.80	0.64
1:M:841:LEU:HD12	1:P:839:VAL:HG13	1.80	0.64
1:h:759:LEU:HD21	1:i:764:LYS:HB3	1.79	0.64
1:X:798:MET:HE1	1:Z:846:PHE:CZ	2.33	0.64
1:A:846:PHE:CZ	1:m:798:MET:HE1	2.33	0.63
1:Y:791:GLU:OE1	1:Z:794:LYS:NZ	2.31	0.63
1:B:794:LYS:NZ	1:C:791:GLU:OE1	2.31	0.63
1:D:791:GLU:OE1	1:E:794:LYS:NZ	2.32	0.62
1:j:798:MET:HE1	1:l:846:PHE:HZ	1.61	0.62
1:Q:761:ARG:O	1:Q:765:VAL:HG23	1.98	0.62
1:e:791:GLU:OE1	1:f:794:LYS:NZ	2.30	0.62
1:F:785:GLN:O	1:F:789:GLU:HG3	2.00	0.61
1:G:839:VAL:HB	1:J:837:THR:HG23	1.81	0.61
1:k:764:LYS:HB3	1:m:759:LEU:HD11	1.80	0.61
1:H:761:ARG:O	1:H:765:VAL:HG23	2.00	0.61
1:G:769:GLU:OE2	1:I:766:ARG:NH2	2.34	0.61
1:Q:812:VAL:O	1:Q:812:VAL:HG23	2.01	0.61
1:j:758:GLU:O	1:j:762:VAL:HG23	1.99	0.61
1:A:846:PHE:HZ	1:m:798:MET:HE1	1.66	0.61
1:B:768:LEU:HD22	1:C:759:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:GLN:O	1:C:789:GLU:HG3	2.01	0.60
1:B:791:GLU:OE1	1:A:794:LYS:NZ	2.34	0.60
1:a:802:LEU:HD23	1:a:807:ILE:HG13	1.83	0.60
1:a:802:LEU:HD21	1:a:810:LEU:CD1	2.33	0.59
1:F:821:LEU:HD21	1:I:842:PHE:HZ	1.67	0.59
1:j:785:GLN:O	1:j:789:GLU:HG3	2.03	0.59
1:S:791:GLU:OE1	1:T:794:LYS:NZ	2.31	0.59
1:V:768:LEU:HD22	1:X:759:LEU:HD13	1.85	0.58
1:m:785:GLN:O	1:m:789:GLU:HG3	2.03	0.58
1:d:825:LEU:HD21	1:e:822:LEU:HB3	1.86	0.58
1:O:785:GLN:O	1:O:789:GLU:HG3	2.03	0.58
1:S:839:VAL:HB	1:V:837:THR:HG23	1.85	0.58
1:R:785:GLN:O	1:R:789:GLU:HG3	2.04	0.58
1:V:764:LYS:HB3	1:X:759:LEU:HD11	1.85	0.58
1:h:768:LEU:HD22	1:j:759:LEU:HD13	1.86	0.58
1:H:812:VAL:HG23	1:H:812:VAL:O	2.04	0.58
1:X:785:GLN:O	1:X:789:GLU:HG3	2.03	0.58
1:d:802:LEU:HD21	1:d:810:LEU:CD1	2.34	0.58
1:g:758:GLU:O	1:g:762:VAL:HG23	2.04	0.57
1:B:839:VAL:HG13	1:k:841:LEU:HD12	1.86	0.57
1:J:841:LEU:HD12	1:M:839:VAL:HG13	1.87	0.57
1:b:841:LEU:HD12	1:e:839:VAL:HG13	1.86	0.57
1:K:815:PRO:O	1:K:819:VAL:HG23	2.04	0.57
1:I:758:GLU:O	1:I:762:VAL:HG23	2.04	0.57
1:X:798:MET:HE1	1:Z:846:PHE:HZ	1.69	0.57
1:Y:841:LEU:HD12	1:b:839:VAL:HG13	1.85	0.57
1:N:761:ARG:O	1:N:765:VAL:HG23	2.04	0.57
1:e:841:LEU:HD12	1:h:839:VAL:HG13	1.87	0.57
1:V:791:GLU:OE1	1:W:794:LYS:NZ	2.37	0.57
1:C:802:LEU:HD21	1:C:810:LEU:CD1	2.35	0.57
1:g:843:ASN:OD1	1:g:853:ALA:HB2	2.05	0.57
1:M:798:MET:HE1	1:O:791:GLU:CD	2.30	0.56
1:V:759:LEU:HD21	1:W:764:LYS:HB3	1.87	0.56
1:D:839:VAL:HB	1:G:837:THR:HG23	1.86	0.56
1:S:765:VAL:O	1:S:769:GLU:HG2	2.04	0.56
1:G:765:VAL:O	1:G:769:GLU:HG2	2.05	0.56
1:P:759:LEU:HD21	1:Q:764:LYS:HB3	1.87	0.56
1:d:802:LEU:HD21	1:d:810:LEU:HD13	1.86	0.56
1:j:802:LEU:HD21	1:j:810:LEU:CD1	2.36	0.56
1:T:761:ARG:O	1:T:765:VAL:HG23	2.05	0.56
1:G:841:LEU:HD12	1:J:839:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:798:MET:HE1	1:R:791:GLU:CD	2.31	0.56
1:S:841:LEU:HD12	1:V:839:VAL:HG13	1.87	0.56
1:O:843:ASN:OD1	1:O:853:ALA:HB2	2.05	0.56
1:f:756:GLU:OE2	1:f:760:GLN:NE2	2.39	0.56
1:J:798:MET:HE1	1:L:791:GLU:CD	2.31	0.56
1:K:817:MET:HE1	1:L:811:ALA:HB1	1.88	0.56
1:k:798:MET:HE1	1:m:791:GLU:CD	2.31	0.56
1:G:798:MET:HE1	1:I:791:GLU:CD	2.31	0.55
1:I:843:ASN:OD1	1:I:853:ALA:HB2	2.07	0.55
1:c:812:VAL:HG23	1:c:812:VAL:O	2.06	0.55
1:R:758:GLU:O	1:R:762:VAL:HG23	2.06	0.55
1:G:791:GLU:OE1	1:H:794:LYS:NZ	2.39	0.55
1:K:762:VAL:O	1:K:766:ARG:HG3	2.06	0.55
1:R:769:GLU:OE1	1:T:766:ARG:NH2	2.40	0.55
1:h:764:LYS:HB3	1:j:759:LEU:HD11	1.87	0.55
1:S:798:MET:HE1	1:U:791:GLU:CD	2.32	0.55
1:k:762:VAL:O	1:k:766:ARG:HG3	2.07	0.55
1:P:791:GLU:OE1	1:Q:794:LYS:NZ	2.34	0.55
1:h:798:MET:HE1	1:j:791:GLU:CD	2.32	0.55
1:D:759:LEU:HD11	1:E:764:LYS:HB3	1.88	0.54
1:O:802:LEU:HD21	1:O:810:LEU:HD13	1.90	0.54
1:O:821:LEU:HD12	1:P:819:VAL:HG23	1.90	0.54
1:h:791:GLU:OE1	1:i:794:LYS:NZ	2.30	0.54
1:k:773:ALA:HB1	1:l:779:LEU:HD21	1.90	0.54
1:M:791:GLU:OE1	1:N:794:LYS:NZ	2.41	0.54
1:j:843:ASN:OD1	1:j:853:ALA:HB2	2.08	0.54
1:E:818:GLN:O	1:E:822:LEU:HG	2.08	0.54
1:h:841:LEU:HD12	1:k:839:VAL:HG13	1.90	0.54
1:j:802:LEU:HD21	1:j:810:LEU:HD13	1.88	0.54
1:d:758:GLU:O	1:d:762:VAL:HG23	2.08	0.54
1:B:764:LYS:HB3	1:C:759:LEU:HD11	1.89	0.53
1:Z:818:GLN:O	1:Z:822:LEU:HG	2.08	0.53
1:b:798:MET:HE1	1:d:791:GLU:CD	2.33	0.53
1:J:756:GLU:OE2	1:J:760:GLN:NE2	2.40	0.53
1:R:843:ASN:OD1	1:R:853:ALA:HB2	2.09	0.53
1:b:791:GLU:OE1	1:c:794:LYS:NZ	2.40	0.53
1:G:759:LEU:HD11	1:H:764:LYS:HB3	1.90	0.53
1:F:821:LEU:HD12	1:G:819:VAL:HG23	1.90	0.53
1:I:825:LEU:HD21	1:J:822:LEU:HB3	1.90	0.53
1:e:798:MET:HE1	1:g:791:GLU:CD	2.34	0.53
1:f:818:GLN:O	1:f:822:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:818:GLN:O	1:c:822:LEU:HG	2.10	0.52
1:l:818:GLN:O	1:l:822:LEU:HG	2.08	0.52
1:C:798:MET:HE1	1:E:846:PHE:CZ	2.44	0.52
1:U:802:LEU:HD21	1:U:810:LEU:CD1	2.39	0.52
1:Y:794:LYS:HE3	1:Y:798:MET:HE3	1.91	0.52
1:Q:818:GLN:O	1:Q:822:LEU:HG	2.10	0.52
1:T:818:GLN:O	1:T:822:LEU:HG	2.09	0.52
1:i:818:GLN:O	1:i:822:LEU:HG	2.09	0.52
1:A:818:GLN:O	1:A:822:LEU:HG	2.09	0.52
1:R:768:LEU:HD12	1:T:759:LEU:HD13	1.92	0.52
1:C:802:LEU:HD21	1:C:810:LEU:HD13	1.92	0.52
1:K:818:GLN:O	1:K:822:LEU:HG	2.09	0.52
1:W:818:GLN:O	1:W:822:LEU:HG	2.08	0.52
1:g:765:VAL:O	1:g:769:GLU:HG2	2.09	0.52
1:V:798:MET:HE1	1:X:791:GLU:CD	2.34	0.52
1:X:765:VAL:O	1:X:769:GLU:HG2	2.09	0.52
1:C:802:LEU:HD23	1:C:807:ILE:HG13	1.92	0.51
1:O:802:LEU:HD21	1:O:810:LEU:CD1	2.40	0.51
1:k:759:LEU:HD11	1:l:765:VAL:HG22	1.91	0.51
1:D:798:MET:HE1	1:F:791:GLU:CD	2.35	0.51
1:I:802:LEU:HD21	1:I:810:LEU:HD13	1.93	0.51
1:V:755:THR:O	1:V:759:LEU:N	2.40	0.51
1:d:768:LEU:HD12	1:f:759:LEU:HD13	1.92	0.51
1:L:825:LEU:HD21	1:M:822:LEU:HB3	1.92	0.51
1:N:818:GLN:O	1:N:822:LEU:HG	2.10	0.51
1:U:802:LEU:HD21	1:U:810:LEU:HD13	1.93	0.51
1:b:768:LEU:HD22	1:d:759:LEU:HD22	1.91	0.51
1:F:798:MET:HE1	1:H:846:PHE:CZ	2.46	0.51
1:J:759:LEU:HD13	1:K:768:LEU:HD22	1.91	0.51
1:B:822:LEU:HB3	1:m:825:LEU:HD21	1.93	0.51
1:D:764:LYS:HB3	1:F:759:LEU:HD11	1.93	0.51
1:Y:759:LEU:HD21	1:Z:764:LYS:HB3	1.94	0.51
1:O:768:LEU:HD22	1:Q:759:LEU:HD12	1.93	0.50
1:Y:755:THR:O	1:Y:759:LEU:N	2.41	0.50
1:B:759:LEU:HD21	1:A:764:LYS:HB3	1.93	0.50
1:H:818:GLN:O	1:H:822:LEU:HG	2.10	0.50
1:P:794:LYS:NZ	1:R:791:GLU:OE2	2.33	0.50
1:j:768:LEU:HD12	1:l:759:LEU:CD1	2.42	0.49
1:l:815:PRO:O	1:l:819:VAL:HG23	2.12	0.49
1:F:822:LEU:HD11	1:F:845:ALA:O	2.13	0.49
1:a:768:LEU:HD12	1:c:759:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:817:MET:HE1	1:m:811:ALA:HB1	1.95	0.49
1:C:825:LEU:HD21	1:D:822:LEU:HB3	1.95	0.48
1:m:843:ASN:OD1	1:m:853:ALA:HB2	2.12	0.48
1:B:822:LEU:HD22	1:m:821:LEU:HD22	1.95	0.48
1:F:802:LEU:HD21	1:F:810:LEU:CD1	2.44	0.48
1:V:773:ALA:HB1	1:W:779:LEU:HD21	1.95	0.48
1:d:768:LEU:HD12	1:f:759:LEU:CD1	2.43	0.48
1:J:773:ALA:HB1	1:K:779:LEU:HD21	1.94	0.48
1:Q:817:MET:HE2	1:Q:817:MET:HA	1.96	0.48
1:T:798:MET:HE1	1:T:827:LEU:HD21	1.96	0.48
1:J:764:LYS:HB3	1:L:759:LEU:HD11	1.95	0.48
1:P:827:LEU:HD21	1:R:831:LEU:CB	2.43	0.48
1:X:812:VAL:HG12	1:X:816:GLU:HB2	1.96	0.48
1:d:802:LEU:HD23	1:d:807:ILE:HG13	1.96	0.48
1:U:802:LEU:HD23	1:U:807:ILE:HG13	1.95	0.48
1:R:768:LEU:HD12	1:T:759:LEU:CD1	2.44	0.47
1:J:759:LEU:HD11	1:K:764:LYS:HB3	1.95	0.47
1:L:785:GLN:O	1:L:789:GLU:HG3	2.13	0.47
1:J:827:LEU:HD21	1:L:831:LEU:CB	2.43	0.47
1:X:843:ASN:OD1	1:X:853:ALA:HB2	2.14	0.47
1:G:827:LEU:HD21	1:I:831:LEU:CB	2.44	0.47
1:I:802:LEU:HD21	1:I:810:LEU:CD1	2.44	0.47
1:j:802:LEU:HD23	1:j:807:ILE:HG13	1.97	0.47
1:m:812:VAL:HG12	1:m:816:GLU:HB2	1.96	0.47
1:g:825:LEU:HD21	1:h:822:LEU:HB3	1.96	0.47
1:k:770:LEU:HD11	1:l:775:ALA:HB1	1.95	0.47
1:J:762:VAL:O	1:J:766:ARG:HG3	2.15	0.47
1:b:762:VAL:O	1:b:766:ARG:HG3	2.15	0.47
1:k:768:LEU:HD22	1:m:759:LEU:HD22	1.97	0.47
1:I:822:LEU:HD11	1:I:845:ALA:O	2.15	0.46
1:Y:827:LEU:HD21	1:a:831:LEU:CB	2.44	0.46
1:d:843:ASN:OD1	1:d:853:ALA:HB2	2.15	0.46
1:B:822:LEU:HD13	1:C:842:PHE:CE1	2.51	0.46
1:Q:762:VAL:O	1:Q:766:ARG:HG3	2.15	0.46
1:g:794:LYS:NZ	1:i:791:GLU:OE2	2.48	0.46
1:C:843:ASN:OD1	1:C:853:ALA:HB2	2.16	0.46
1:E:810:LEU:O	1:E:818:GLN:NE2	2.49	0.46
1:R:794:LYS:O	1:R:798:MET:HG3	2.14	0.46
1:L:794:LYS:NZ	1:N:791:GLU:OE1	2.45	0.46
1:g:812:VAL:HG12	1:g:816:GLU:HB2	1.97	0.46
1:D:827:LEU:HD21	1:F:831:LEU:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:768:LEU:HD22	1:W:759:LEU:HD12	1.98	0.46
1:j:768:LEU:HD12	1:l:759:LEU:HD13	1.97	0.46
1:m:822:LEU:HD11	1:m:845:ALA:O	2.15	0.46
1:O:812:VAL:HG12	1:O:816:GLU:HB2	1.98	0.46
1:a:812:VAL:HG12	1:a:816:GLU:HB2	1.98	0.46
1:e:827:LEU:HD21	1:g:831:LEU:CB	2.44	0.45
1:D:773:ALA:HB1	1:E:779:LEU:HD21	1.99	0.45
1:U:768:LEU:HD22	1:W:759:LEU:CD1	2.46	0.45
1:I:821:LEU:HD22	1:J:822:LEU:HD22	1.98	0.45
1:L:762:VAL:HG12	1:L:766:ARG:HD2	1.98	0.45
1:k:827:LEU:HD21	1:m:831:LEU:CB	2.44	0.45
1:b:827:LEU:HD21	1:d:831:LEU:CB	2.44	0.45
1:B:798:MET:HE1	1:C:791:GLU:CD	2.41	0.45
1:M:822:LEU:HD13	1:O:842:PHE:CE1	2.52	0.45
1:O:798:MET:HE1	1:Q:846:PHE:CZ	2.51	0.45
1:a:802:LEU:HD21	1:a:810:LEU:HD13	1.97	0.45
1:j:825:LEU:HD21	1:k:822:LEU:HB3	1.99	0.45
1:O:768:LEU:HD22	1:Q:759:LEU:CD1	2.46	0.45
1:b:766:ARG:HD2	1:c:772:TYR:CG	2.52	0.45
1:M:827:LEU:HD21	1:O:831:LEU:CB	2.44	0.45
1:U:783:LYS:HA	1:W:777:LEU:HD11	1.99	0.45
1:i:810:LEU:O	1:i:818:GLN:NE2	2.50	0.45
1:C:794:LYS:O	1:C:798:MET:HG3	2.17	0.45
1:L:794:LYS:O	1:L:798:MET:HG3	2.17	0.45
1:U:793:LYS:O	1:U:797:GLN:HG3	2.17	0.44
1:h:755:THR:O	1:h:759:LEU:N	2.42	0.44
1:S:827:LEU:HD21	1:U:831:LEU:CB	2.45	0.44
1:d:783:LYS:HA	1:f:777:LEU:HD11	1.99	0.44
1:R:825:LEU:HD21	1:S:822:LEU:HB3	1.99	0.44
1:e:759:LEU:HD21	1:f:764:LYS:HB3	1.98	0.44
1:f:817:MET:HE1	1:g:811:ALA:HB1	1.99	0.44
1:M:817:MET:HE3	1:O:812:VAL:HG13	1.99	0.44
1:a:798:MET:HE1	1:c:846:PHE:CZ	2.53	0.44
1:e:762:VAL:O	1:e:766:ARG:HG3	2.18	0.44
1:X:772:TYR:CG	1:Z:766:ARG:HD2	2.53	0.44
1:h:827:LEU:HD21	1:j:831:LEU:CB	2.46	0.44
1:F:798:MET:HE1	1:H:846:PHE:HZ	1.83	0.44
1:I:812:VAL:HG12	1:I:816:GLU:HB2	2.00	0.44
1:V:762:VAL:O	1:V:766:ARG:HG3	2.18	0.44
1:Y:798:MET:HE1	1:a:791:GLU:CD	2.43	0.44
1:j:794:LYS:O	1:j:798:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:812:VAL:HG12	1:F:816:GLU:HB2	2.00	0.44
1:b:794:LYS:NZ	1:d:791:GLU:OE1	2.42	0.44
1:J:822:LEU:HD13	1:L:842:PHE:CE1	2.53	0.44
1:B:773:ALA:HB1	1:A:779:LEU:HD21	2.00	0.43
1:a:768:LEU:HD12	1:c:759:LEU:CD1	2.46	0.43
1:R:772:TYR:CG	1:T:766:ARG:HD2	2.53	0.43
1:S:794:LYS:NZ	1:U:791:GLU:OE1	2.44	0.43
1:X:825:LEU:HD21	1:Y:822:LEU:HB3	2.00	0.43
1:Y:794:LYS:NZ	1:a:791:GLU:OE1	2.34	0.43
1:k:759:LEU:HG	1:l:768:LEU:HD12	2.00	0.43
1:L:772:TYR:CG	1:N:766:ARG:HD2	2.53	0.43
1:B:827:LEU:HD21	1:C:831:LEU:CB	2.46	0.43
1:G:840:ASN:ND2	1:J:840:ASN:OD1	2.52	0.43
1:c:810:LEU:O	1:c:818:GLN:NE2	2.52	0.43
1:D:767:GLU:O	1:D:771:VAL:HG23	2.19	0.43
1:N:762:VAL:O	1:N:766:ARG:HG3	2.19	0.43
1:U:772:TYR:CG	1:W:766:ARG:HD2	2.54	0.43
1:j:772:TYR:CG	1:l:766:ARG:HD2	2.53	0.43
1:O:825:LEU:HD21	1:P:822:LEU:HB3	2.00	0.43
1:e:756:GLU:OE2	1:e:760:GLN:NE2	2.52	0.43
1:Z:762:VAL:O	1:Z:766:ARG:HG3	2.19	0.43
1:d:812:VAL:HG12	1:d:816:GLU:HB2	2.01	0.43
1:l:762:VAL:O	1:l:766:ARG:HG3	2.18	0.43
1:O:821:LEU:HD11	1:P:818:GLN:HB3	2.01	0.42
1:T:810:LEU:O	1:T:818:GLN:NE2	2.51	0.42
1:a:825:LEU:HD21	1:b:822:LEU:HB3	2.00	0.42
1:g:772:TYR:CG	1:i:766:ARG:HD2	2.54	0.42
1:Z:810:LEU:O	1:Z:818:GLN:NE2	2.51	0.42
1:d:794:LYS:O	1:d:798:MET:HG3	2.18	0.42
1:H:810:LEU:O	1:H:818:GLN:NE2	2.52	0.42
1:L:821:LEU:HD21	1:O:842:PHE:HZ	1.84	0.42
1:P:764:LYS:HB3	1:R:759:LEU:HD11	2.01	0.42
1:U:825:LEU:HD21	1:V:822:LEU:HB3	2.01	0.42
1:F:802:LEU:HD21	1:F:810:LEU:HD13	2.01	0.42
1:S:840:ASN:ND2	1:V:840:ASN:OD1	2.52	0.42
1:D:794:LYS:NZ	1:F:791:GLU:OE1	2.45	0.42
1:G:837:THR:HG22	1:G:838:PRO:O	2.20	0.42
1:d:816:GLU:OE2	1:d:820:LYS:NZ	2.53	0.42
1:h:839:VAL:HB	1:k:837:THR:OG1	2.19	0.42
1:A:759:LEU:CD1	1:m:768:LEU:HD12	2.50	0.42
1:A:766:ARG:HD2	1:m:772:TYR:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:837:THR:HG22	1:V:838:PRO:O	2.19	0.42
1:e:840:ASN:ND2	1:h:840:ASN:OD1	2.53	0.42
1:A:840:ASN:OD1	1:A:840:ASN:N	2.45	0.42
1:C:812:VAL:HG12	1:C:816:GLU:HB2	2.02	0.42
1:I:802:LEU:HD23	1:I:807:ILE:HG13	2.02	0.42
1:h:840:ASN:ND2	1:k:840:ASN:OD1	2.53	0.42
1:j:783:LYS:HA	1:l:777:LEU:HD11	2.02	0.42
1:U:810:LEU:HD23	1:W:811:ALA:HB2	2.02	0.42
1:e:839:VAL:HB	1:h:837:THR:OG1	2.20	0.42
1:g:794:LYS:CE	1:i:791:GLU:OE2	2.68	0.42
1:i:817:MET:HE2	1:i:817:MET:HA	2.01	0.42
1:N:810:LEU:O	1:N:818:GLN:NE2	2.51	0.41
1:h:793:LYS:O	1:h:797:GLN:HG3	2.20	0.41
1:W:810:LEU:HD21	1:W:821:LEU:HD13	2.02	0.41
1:c:762:VAL:O	1:c:766:ARG:CG	2.69	0.41
1:d:821:LEU:HD22	1:e:822:LEU:HD22	2.02	0.41
1:C:829:SER:OG	1:D:830:THR:HB	2.20	0.41
1:M:766:ARG:O	1:M:770:LEU:HD23	2.21	0.41
1:Y:756:GLU:OE2	1:Y:760:GLN:NE2	2.53	0.41
1:Y:840:ASN:ND2	1:b:840:ASN:OD1	2.53	0.41
1:f:840:ASN:OD1	1:f:840:ASN:N	2.46	0.41
1:j:812:VAL:HG12	1:j:816:GLU:HB2	2.02	0.41
1:k:808:LYS:O	1:k:812:VAL:HG13	2.20	0.41
1:F:821:LEU:HD21	1:I:842:PHE:CZ	2.53	0.41
1:T:805:SER:O	1:T:808:LYS:HG3	2.20	0.41
1:V:840:ASN:ND2	1:Y:840:ASN:OD1	2.54	0.41
1:X:768:LEU:HD12	1:Z:759:LEU:HD13	2.02	0.41
1:X:821:LEU:HD22	1:Y:822:LEU:HD12	2.02	0.41
1:h:791:GLU:OE2	1:i:798:MET:HE1	2.20	0.41
1:H:805:SER:O	1:H:808:LYS:HG3	2.21	0.41
1:O:827:LEU:O	1:O:828:LYS:HE3	2.21	0.41
1:P:755:THR:O	1:P:759:LEU:N	2.44	0.41
1:X:783:LYS:HA	1:Z:777:LEU:HD11	2.01	0.41
1:Y:839:VAL:HB	1:b:837:THR:OG1	2.20	0.41
1:g:798:MET:HE1	1:i:846:PHE:CZ	2.55	0.41
1:L:810:LEU:HD23	1:N:811:ALA:HB2	2.02	0.41
1:a:794:LYS:O	1:a:798:MET:HG3	2.21	0.41
1:G:767:GLU:O	1:G:771:VAL:HG23	2.21	0.41
1:I:810:LEU:HD23	1:K:811:ALA:HB2	2.02	0.41
1:Y:773:ALA:HB1	1:Z:779:LEU:HD21	2.02	0.41
1:B:840:ASN:ND2	1:D:840:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:768:LEU:HD22	1:L:759:LEU:HD13	2.02	0.41
1:P:839:VAL:HB	1:S:837:THR:OG1	2.21	0.41
1:Z:840:ASN:OD1	1:Z:840:ASN:N	2.44	0.41
1:B:839:VAL:HB	1:D:837:THR:OG1	2.20	0.41
1:B:840:ASN:OD1	1:k:840:ASN:ND2	2.54	0.41
1:H:840:ASN:OD1	1:H:840:ASN:N	2.44	0.41
1:P:840:ASN:ND2	1:S:840:ASN:OD1	2.53	0.41
1:S:759:LEU:HD21	1:T:765:VAL:HG22	2.02	0.41
1:S:773:ALA:HB1	1:T:779:LEU:HD21	2.01	0.41
1:U:798:MET:HE1	1:W:846:PHE:CZ	2.56	0.41
1:V:767:GLU:O	1:V:771:VAL:HG23	2.21	0.41
1:W:762:VAL:O	1:W:766:ARG:HG3	2.21	0.41
1:b:840:ASN:ND2	1:e:840:ASN:OD1	2.54	0.41
1:k:807:ILE:HG23	1:l:821:LEU:HD11	2.02	0.41
1:D:840:ASN:ND2	1:G:840:ASN:OD1	2.54	0.41
1:E:805:SER:O	1:E:808:LYS:HG3	2.21	0.41
1:U:758:GLU:O	1:U:762:VAL:HG23	2.21	0.41
1:Y:756:GLU:OE2	1:Y:760:GLN:CD	2.64	0.41
1:l:810:LEU:O	1:l:818:GLN:NE2	2.52	0.41
1:G:794:LYS:NZ	1:I:791:GLU:OE1	2.46	0.40
1:K:810:LEU:O	1:K:818:GLN:NE2	2.54	0.40
1:M:756:GLU:OE2	1:M:760:GLN:NE2	2.54	0.40
1:a:821:LEU:HD22	1:b:822:LEU:HD12	2.03	0.40
1:A:810:LEU:O	1:A:818:GLN:NE2	2.54	0.40
1:G:755:THR:O	1:G:759:LEU:N	2.44	0.40
1:K:805:SER:O	1:K:808:LYS:HG3	2.21	0.40
1:G:764:LYS:HB3	1:I:759:LEU:HD11	2.03	0.40
1:L:768:LEU:HD12	1:N:759:LEU:HD13	2.03	0.40
1:M:840:ASN:ND2	1:P:840:ASN:OD1	2.54	0.40
1:V:766:ARG:HD2	1:W:772:TYR:CG	2.56	0.40
1:W:805:SER:O	1:W:808:LYS:HG3	2.22	0.40
1:c:762:VAL:O	1:c:766:ARG:HG2	2.21	0.40
1:E:762:VAL:O	1:E:766:ARG:CG	2.69	0.40
1:b:837:THR:O	1:b:837:THR:HG23	2.22	0.40
1:b:839:VAL:HB	1:e:837:THR:OG1	2.22	0.40
1:g:783:LYS:HA	1:i:777:LEU:HD11	2.02	0.40
1:M:768:LEU:HD21	1:O:762:VAL:HG13	2.04	0.40
1:U:794:LYS:O	1:U:798:MET:HG3	2.21	0.40
1:e:773:ALA:HB1	1:f:779:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	83/140 (59%)	79 (95%)	4 (5%)	0	100	100
1	B	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	C	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	D	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	E	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	F	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	G	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	H	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	I	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	J	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	K	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	L	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	M	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	N	83/140 (59%)	79 (95%)	4 (5%)	0	100	100
1	O	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	P	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	Q	83/140 (59%)	79 (95%)	4 (5%)	0	100	100
1	R	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	S	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	T	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	U	102/140 (73%)	102 (100%)	0	0	100	100
1	V	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	W	83/140 (59%)	79 (95%)	4 (5%)	0	100	100
1	X	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	Y	88/140 (63%)	86 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	a	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	b	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	c	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	d	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	e	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	f	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	g	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	h	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	i	83/140 (59%)	80 (96%)	3 (4%)	0	100	100
1	j	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
1	k	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
1	l	83/140 (59%)	79 (95%)	4 (5%)	0	100	100
1	m	102/140 (73%)	101 (99%)	1 (1%)	0	100	100
All	All	3549/5460 (65%)	3467 (98%)	82 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	68/111 (61%)	64 (94%)	4 (6%)	18	18
1	B	74/111 (67%)	68 (92%)	6 (8%)	11	9
1	C	85/111 (77%)	81 (95%)	4 (5%)	23	26
1	D	74/111 (67%)	69 (93%)	5 (7%)	14	14
1	E	68/111 (61%)	65 (96%)	3 (4%)	25	29
1	F	85/111 (77%)	81 (95%)	4 (5%)	23	26
1	G	74/111 (67%)	69 (93%)	5 (7%)	14	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	68/111 (61%)	63 (93%)	5 (7%)	13	11
1	I	85/111 (77%)	81 (95%)	4 (5%)	23	26
1	J	74/111 (67%)	69 (93%)	5 (7%)	14	14
1	K	68/111 (61%)	65 (96%)	3 (4%)	25	29
1	L	85/111 (77%)	81 (95%)	4 (5%)	23	26
1	M	74/111 (67%)	72 (97%)	2 (3%)	39	49
1	N	68/111 (61%)	62 (91%)	6 (9%)	9	7
1	O	85/111 (77%)	81 (95%)	4 (5%)	23	26
1	P	74/111 (67%)	71 (96%)	3 (4%)	27	33
1	Q	68/111 (61%)	62 (91%)	6 (9%)	9	7
1	R	85/111 (77%)	81 (95%)	4 (5%)	23	26
1	S	74/111 (67%)	71 (96%)	3 (4%)	27	33
1	T	68/111 (61%)	63 (93%)	5 (7%)	13	11
1	U	85/111 (77%)	80 (94%)	5 (6%)	18	18
1	V	74/111 (67%)	68 (92%)	6 (8%)	11	9
1	W	68/111 (61%)	63 (93%)	5 (7%)	13	11
1	X	85/111 (77%)	82 (96%)	3 (4%)	32	39
1	Y	74/111 (67%)	68 (92%)	6 (8%)	11	9
1	Z	68/111 (61%)	63 (93%)	5 (7%)	13	11
1	a	85/111 (77%)	79 (93%)	6 (7%)	13	12
1	b	74/111 (67%)	69 (93%)	5 (7%)	14	14
1	c	68/111 (61%)	61 (90%)	7 (10%)	7	5
1	d	85/111 (77%)	82 (96%)	3 (4%)	32	39
1	e	74/111 (67%)	70 (95%)	4 (5%)	20	21
1	f	68/111 (61%)	64 (94%)	4 (6%)	18	18
1	g	85/111 (77%)	80 (94%)	5 (6%)	18	18
1	h	74/111 (67%)	69 (93%)	5 (7%)	14	14
1	i	68/111 (61%)	64 (94%)	4 (6%)	18	18
1	j	85/111 (77%)	81 (95%)	4 (5%)	23	26
1	k	74/111 (67%)	70 (95%)	4 (5%)	20	21
1	l	68/111 (61%)	63 (93%)	5 (7%)	13	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	m	85/111 (77%)	81 (95%)	4 (5%)	23	26
All	All	2951/4329 (68%)	2776 (94%)	175 (6%)	19	18

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	762	VAL
1	B	768	LEU
1	B	770	LEU
1	B	778	GLU
1	B	796	LYS
1	B	828	LYS
1	A	762	VAL
1	A	796	LYS
1	A	808	LYS
1	A	821	LEU
1	C	756	GLU
1	C	769	GLU
1	C	779	LEU
1	C	821	LEU
1	D	768	LEU
1	D	778	GLU
1	D	796	LYS
1	D	817	MET
1	D	828	LYS
1	E	796	LYS
1	E	808	LYS
1	E	824	SER
1	F	759	LEU
1	F	762	VAL
1	F	769	GLU
1	F	843	ASN
1	G	762	VAL
1	G	768	LEU
1	G	778	GLU
1	G	796	LYS
1	G	828	LYS
1	H	762	VAL
1	H	796	LYS
1	H	807	ILE
1	H	808	LYS
1	H	824	SER

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Mol	Chain	Res	Type
1	I	756	GLU
1	I	759	LEU
1	I	779	LEU
1	I	821	LEU
1	J	759	LEU
1	J	762	VAL
1	J	796	LYS
1	J	817	MET
1	J	828	LYS
1	K	762	VAL
1	K	796	LYS
1	K	808	LYS
1	L	759	LEU
1	L	769	GLU
1	L	779	LEU
1	L	843	ASN
1	M	762	VAL
1	M	796	LYS
1	N	760	GLN
1	N	762	VAL
1	N	766	ARG
1	N	796	LYS
1	N	817	MET
1	N	824	SER
1	O	759	LEU
1	O	769	GLU
1	O	779	LEU
1	O	817	MET
1	P	796	LYS
1	P	817	MET
1	P	828	LYS
1	Q	762	VAL
1	Q	793	LYS
1	Q	796	LYS
1	Q	808	LYS
1	Q	821	LEU
1	Q	824	SER
1	R	759	LEU
1	R	769	GLU
1	R	779	LEU
1	R	821	LEU
1	S	762	VAL

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Mol	Chain	Res	Type
1	S	796	LYS
1	S	828	LYS
1	T	762	VAL
1	T	796	LYS
1	T	808	LYS
1	T	821	LEU
1	T	824	SER
1	U	756	GLU
1	U	759	LEU
1	U	779	LEU
1	U	821	LEU
1	U	843	ASN
1	V	762	VAL
1	V	770	LEU
1	V	778	GLU
1	V	796	LYS
1	V	817	MET
1	V	828	LYS
1	W	762	VAL
1	W	796	LYS
1	W	808	LYS
1	W	817	MET
1	W	821	LEU
1	X	756	GLU
1	X	759	LEU
1	X	821	LEU
1	Y	759	LEU
1	Y	762	VAL
1	Y	768	LEU
1	Y	796	LYS
1	Y	817	MET
1	Y	828	LYS
1	Z	762	VAL
1	Z	766	ARG
1	Z	796	LYS
1	Z	808	LYS
1	Z	824	SER
1	a	756	GLU
1	a	759	LEU
1	a	769	GLU
1	a	779	LEU
1	a	821	LEU

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Mol	Chain	Res	Type
1	a	843	ASN
1	b	762	VAL
1	b	778	GLU
1	b	796	LYS
1	b	817	MET
1	b	828	LYS
1	c	762	VAL
1	c	766	ARG
1	c	793	LYS
1	c	796	LYS
1	c	808	LYS
1	c	821	LEU
1	c	824	SER
1	d	769	GLU
1	d	779	LEU
1	d	821	LEU
1	e	762	VAL
1	e	766	ARG
1	e	796	LYS
1	e	828	LYS
1	f	762	VAL
1	f	766	ARG
1	f	796	LYS
1	f	808	LYS
1	g	756	GLU
1	g	759	LEU
1	g	779	LEU
1	g	817	MET
1	g	821	LEU
1	h	762	VAL
1	h	778	GLU
1	h	796	LYS
1	h	817	MET
1	h	828	LYS
1	i	762	VAL
1	i	796	LYS
1	i	808	LYS
1	i	824	SER
1	j	759	LEU
1	j	769	GLU
1	j	779	LEU
1	j	821	LEU

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Mol	Chain	Res	Type
1	k	762	VAL
1	k	778	GLU
1	k	796	LYS
1	k	828	LYS
1	l	762	VAL
1	l	766	ARG
1	l	796	LYS
1	l	808	LYS
1	l	824	SER
1	m	759	LEU
1	m	762	VAL
1	m	769	GLU
1	m	821	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	840	ASN
1	C	797	GLN
1	D	840	ASN
1	F	840	ASN
1	G	840	ASN
1	H	776	GLN
1	I	797	GLN
1	J	840	ASN
1	L	797	GLN
1	M	840	ASN
1	P	840	ASN
1	S	840	ASN
1	T	760	GLN
1	U	776	GLN
1	U	797	GLN
1	V	840	ASN
1	Y	840	ASN
1	b	840	ASN
1	d	776	GLN
1	d	797	GLN
1	e	840	ASN
1	g	840	ASN
1	h	840	ASN
1	j	797	GLN
1	k	840	ASN

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Mol	Chain	Res	Type
1	l	776	GLN
1	m	776	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.

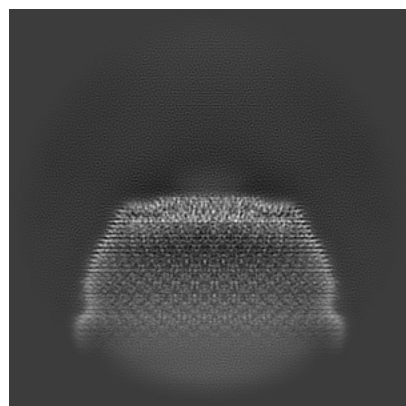
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73819. These allow visual inspection of the internal detail of the map and identification of artifacts.

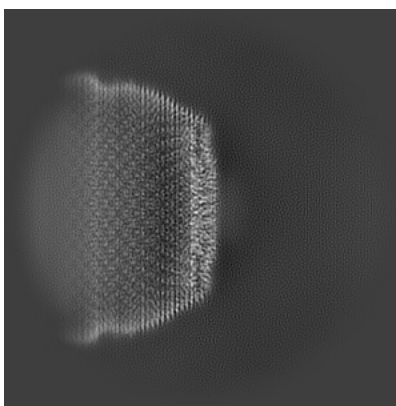
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

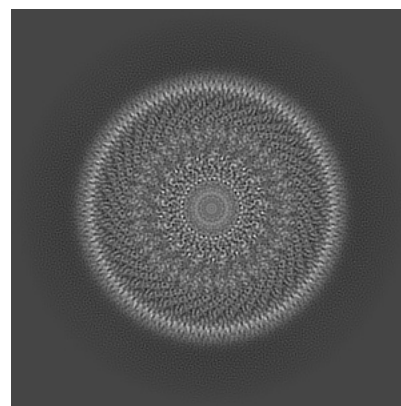
6.1.1 Primary map



X

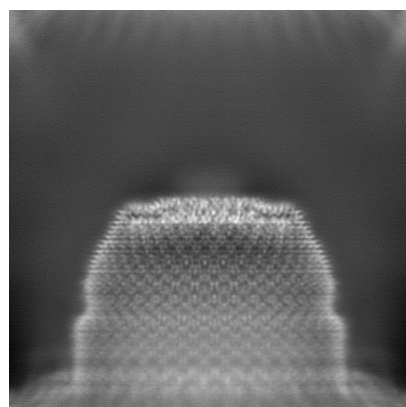


Y

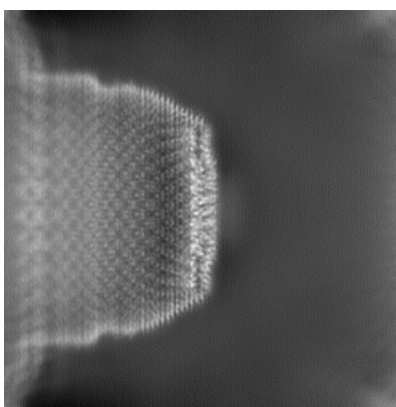


Z

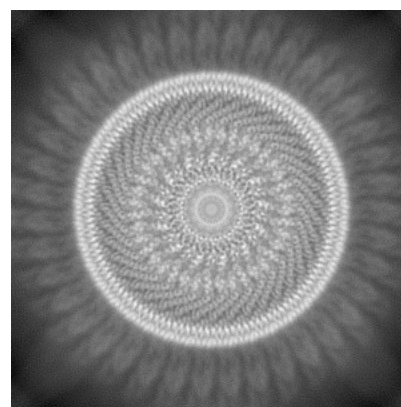
6.1.2 Raw map



X



Y

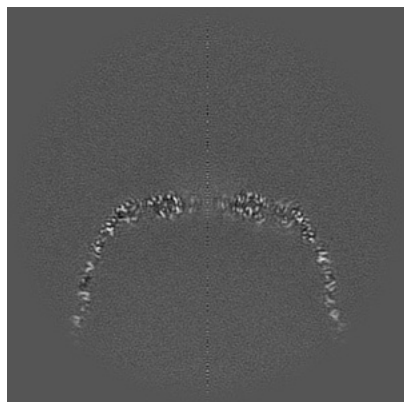


Z

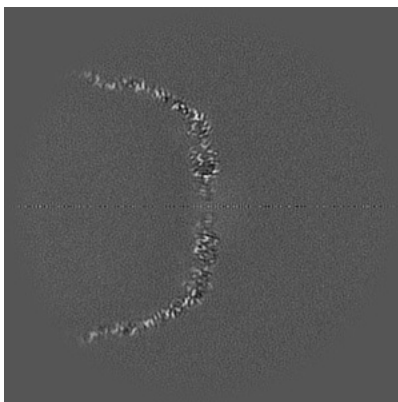
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

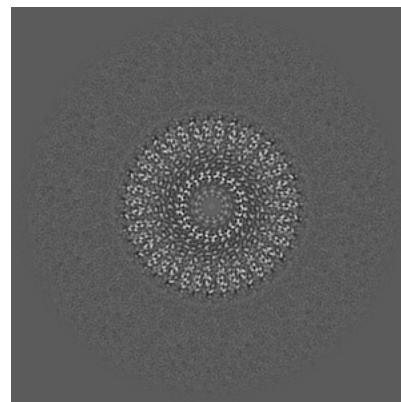
6.2.1 Primary map



X Index: 192

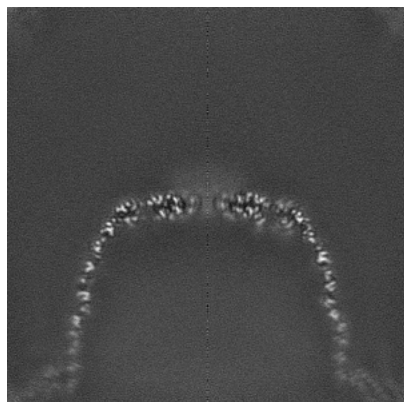


Y Index: 192

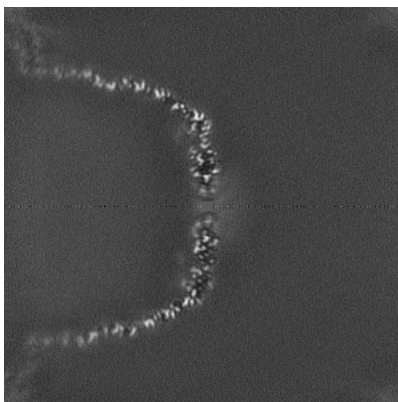


Z Index: 192

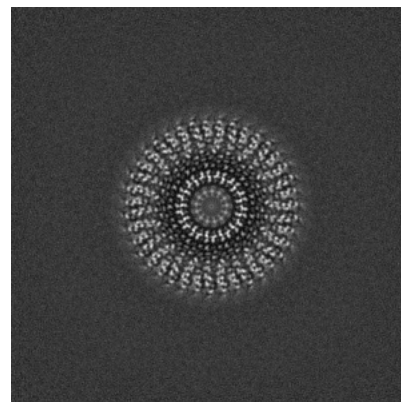
6.2.2 Raw map



X Index: 192



Y Index: 192

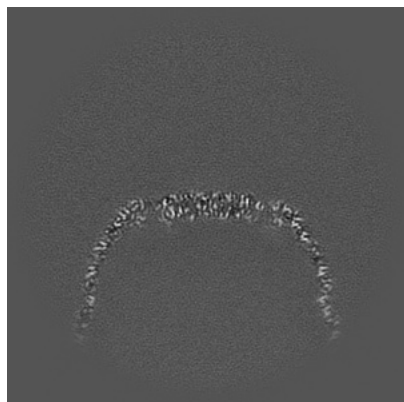


Z Index: 192

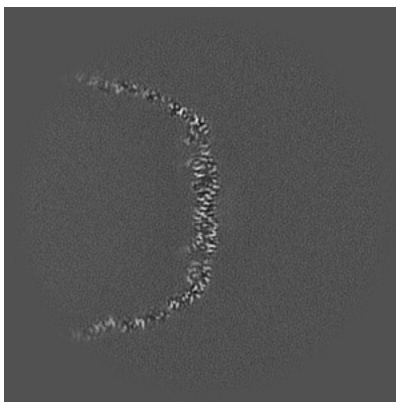
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

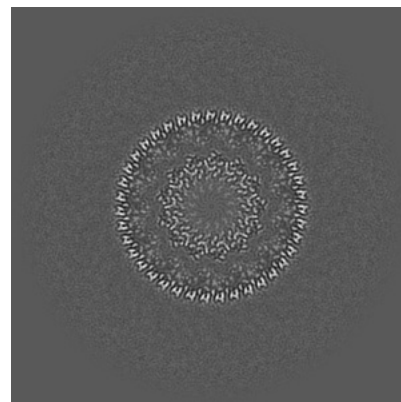
6.3.1 Primary map



X Index: 224

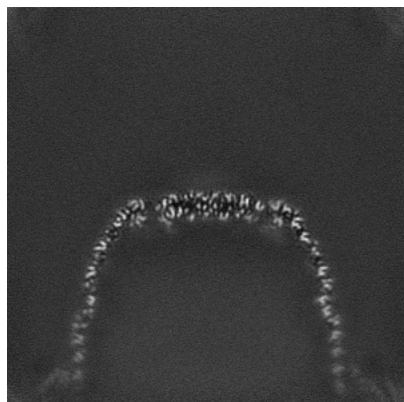


Y Index: 220

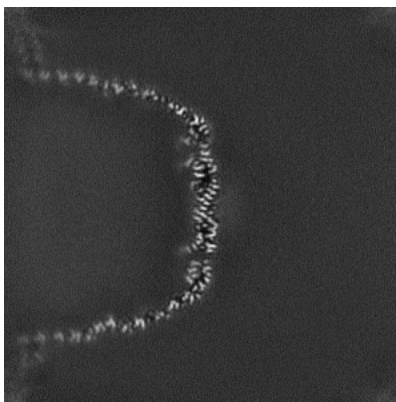


Z Index: 184

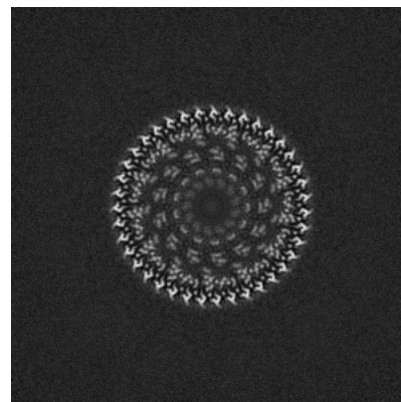
6.3.2 Raw map



X Index: 224



Y Index: 220

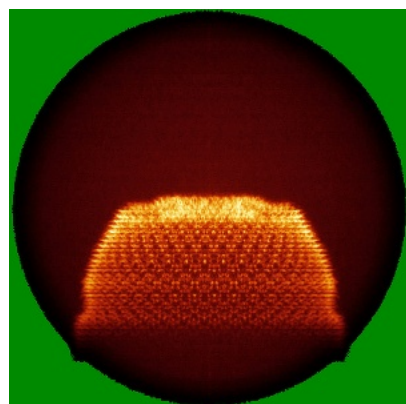


Z Index: 180

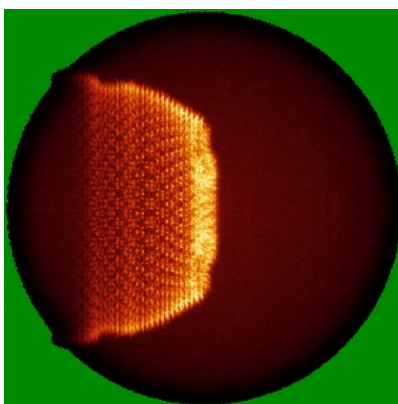
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

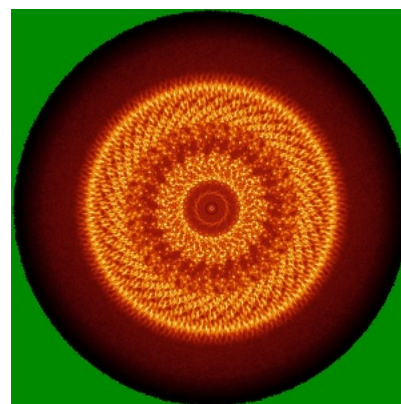
6.4.1 Primary map



X

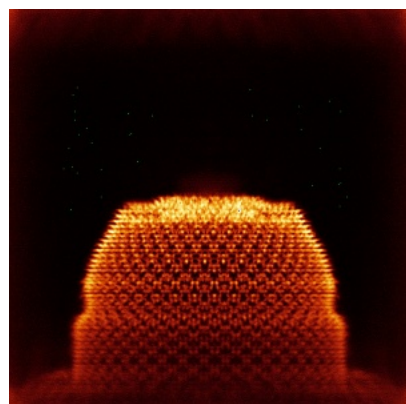


Y

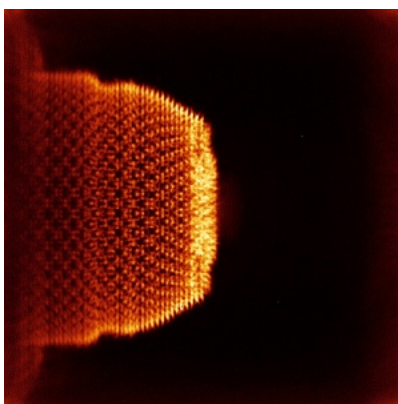


Z

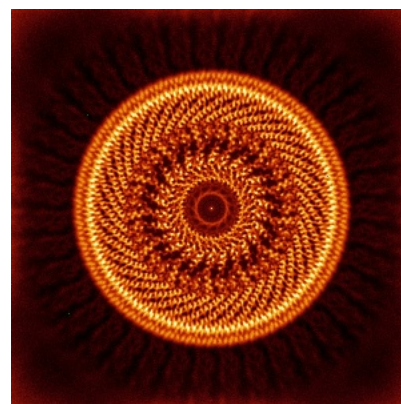
6.4.2 Raw map



X



Y

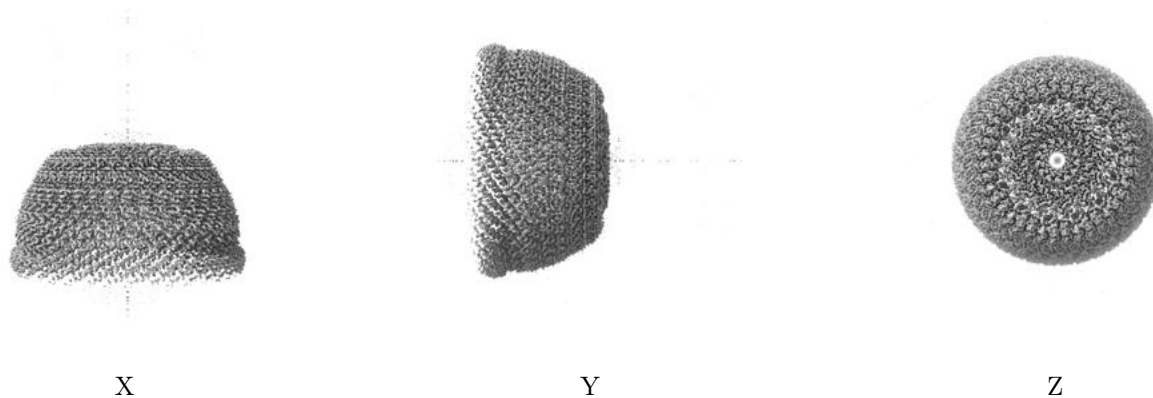


Z

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.

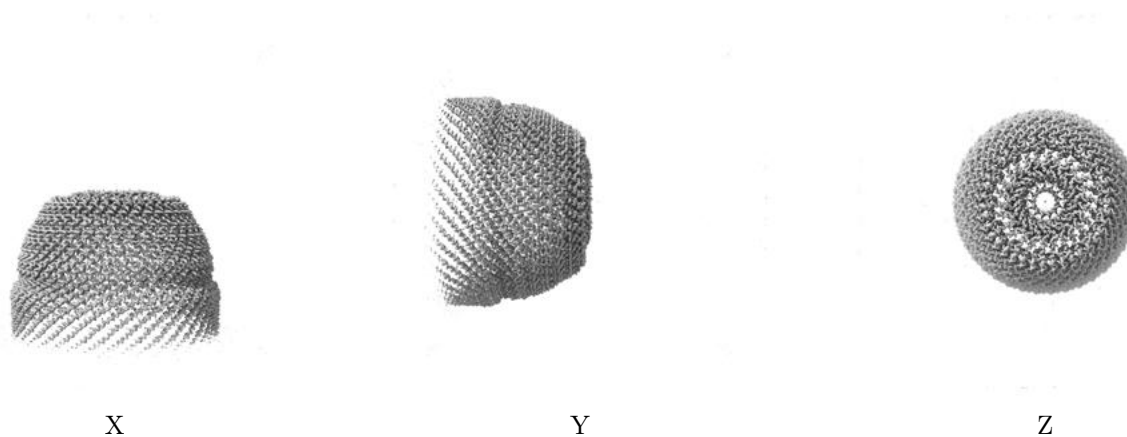
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0615. 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.

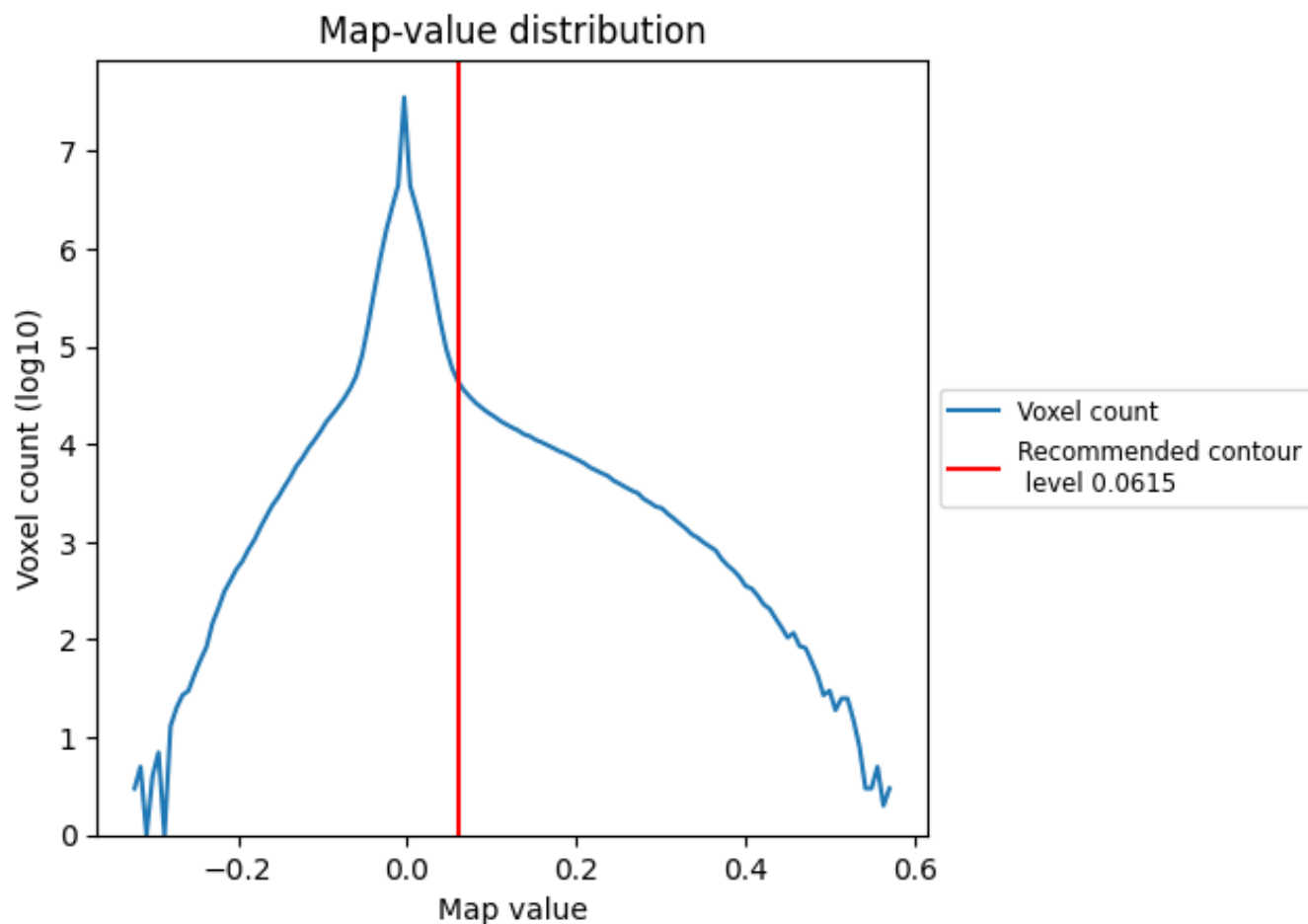
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

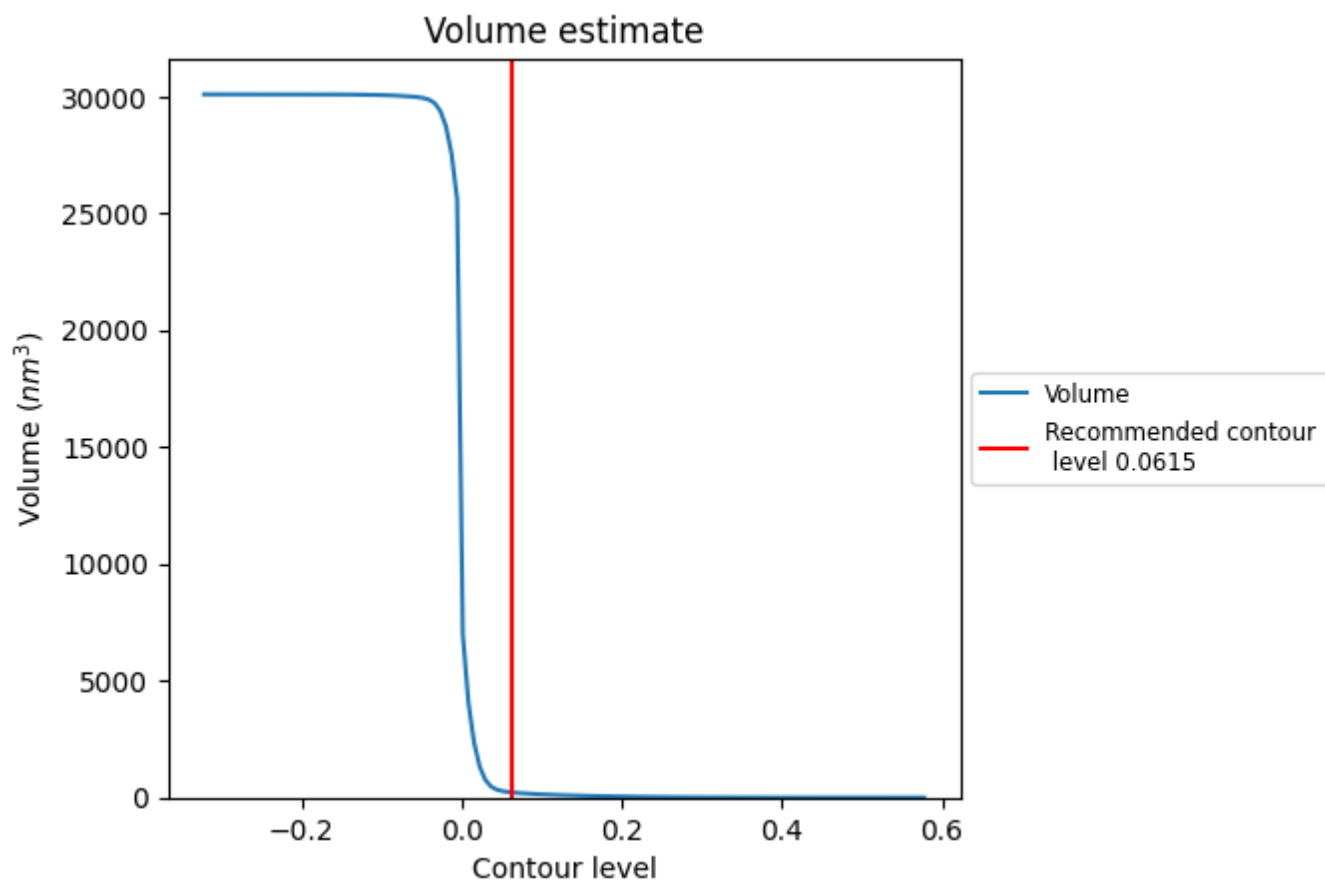
This section contains the results of statistical analysis of the map.

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.

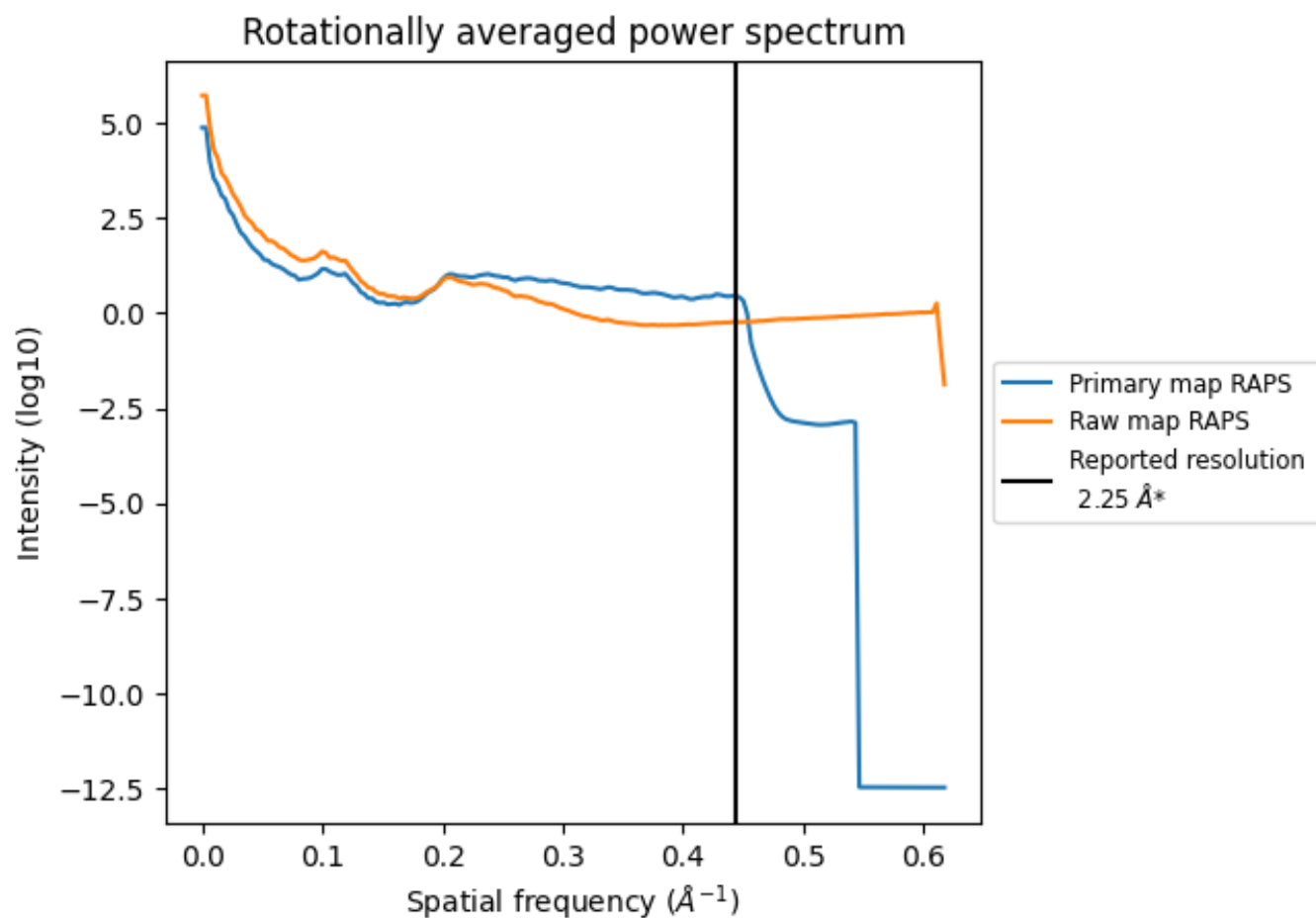
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm³; this corresponds to an approximate mass of 203 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

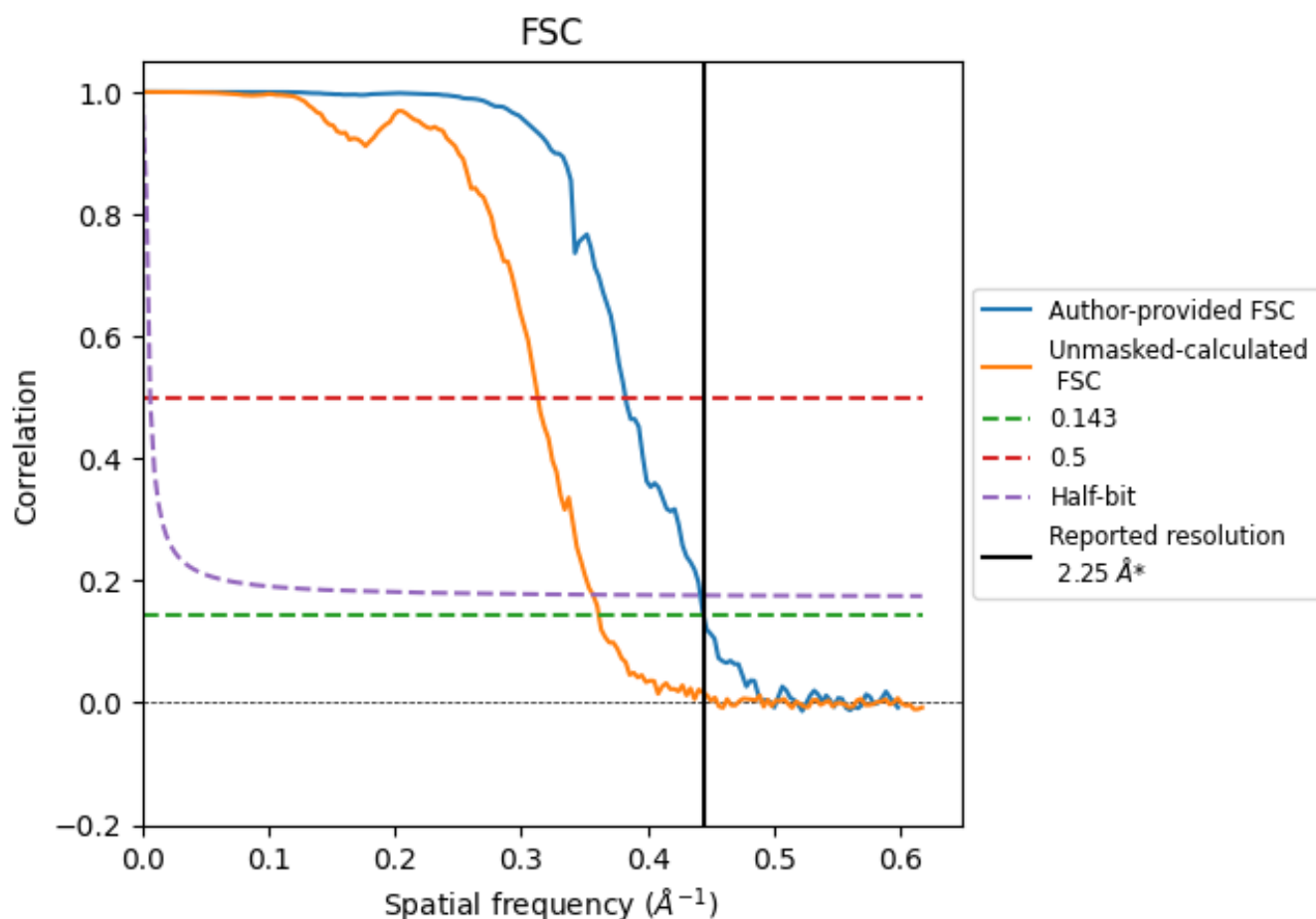


*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.444 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

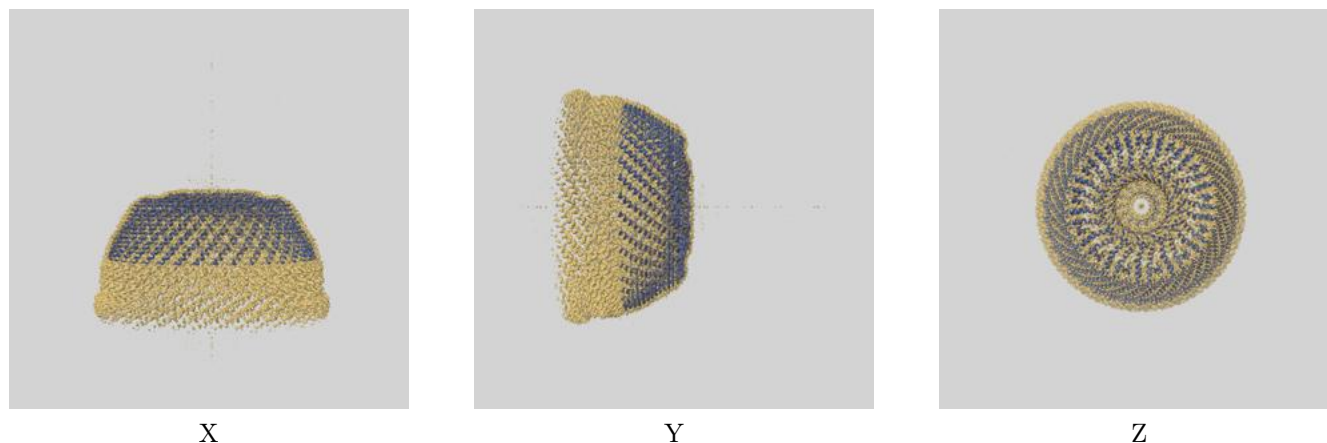
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.61	2.26
Unmasked-calculated*	2.77	3.19	2.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.77 differs from the reported value 2.25 by more than 10 %

9 Map-model fit [i](#)

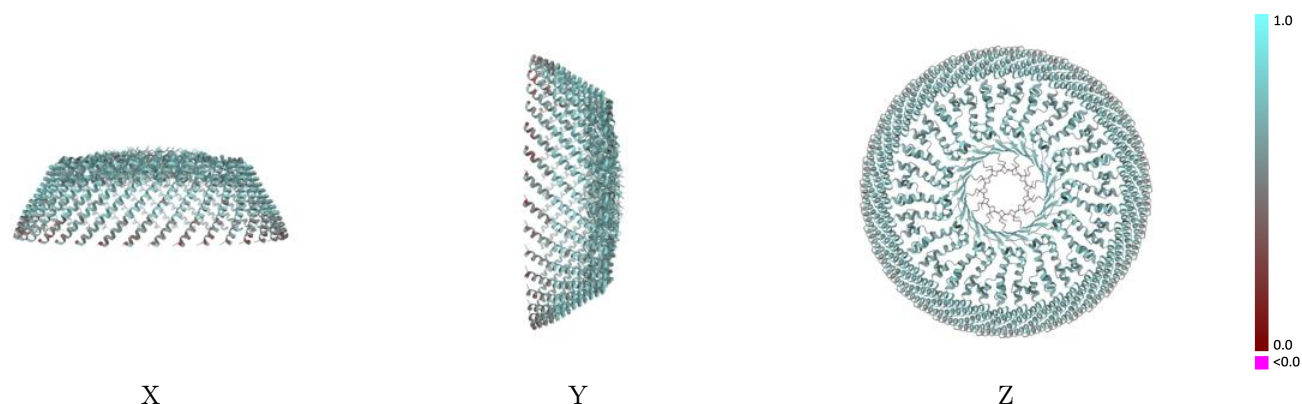
This section contains information regarding the fit between EMDB map EMD-73819 and PDB model 9Z5N. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



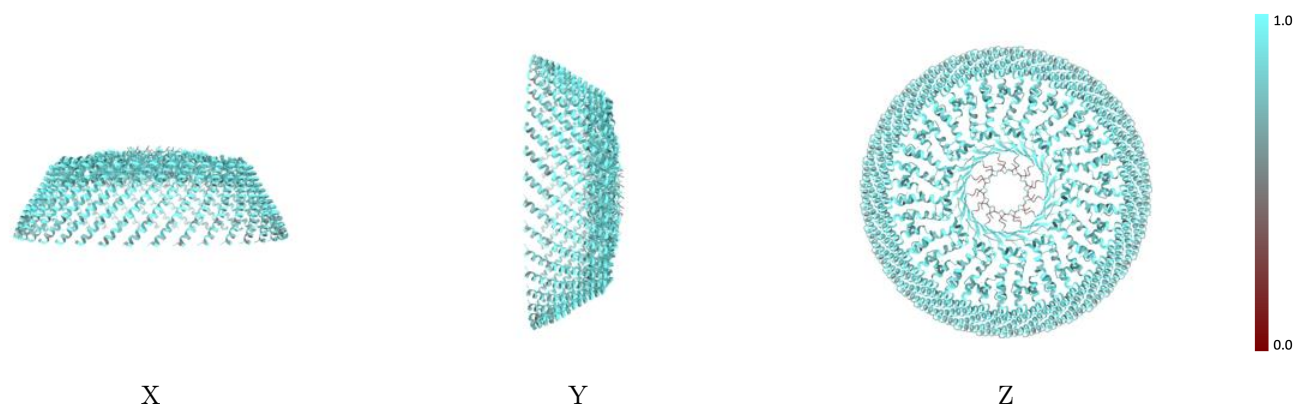
The images above show the 3D surface view of the map at the recommended contour level 0.0615 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



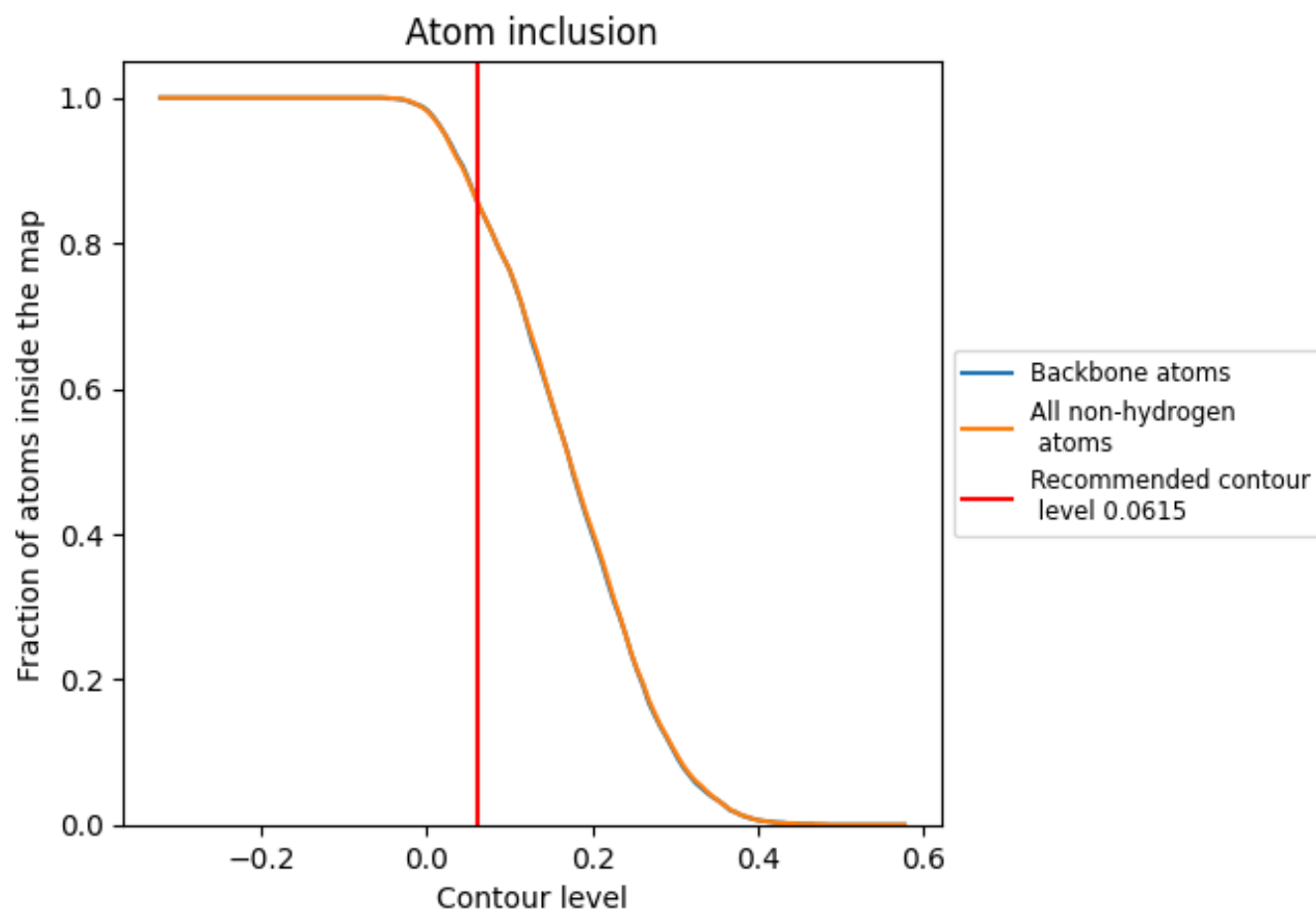
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0615).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.0615) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.6200
A	 0.8650	 0.6090
B	 0.8450	 0.6070
C	 0.8860	 0.6390
D	 0.8430	 0.6040
E	 0.8580	 0.6030
F	 0.8830	 0.6420
G	 0.8420	 0.6110
H	 0.8620	 0.6030
I	 0.8830	 0.6410
J	 0.8430	 0.6090
K	 0.8610	 0.6070
L	 0.8910	 0.6420
M	 0.8420	 0.6060
N	 0.8640	 0.6060
O	 0.8850	 0.6460
P	 0.8360	 0.6110
Q	 0.8520	 0.5980
R	 0.8820	 0.6450
S	 0.8330	 0.6080
T	 0.8620	 0.6100
U	 0.8910	 0.6410
V	 0.8370	 0.6080
W	 0.8650	 0.6090
X	 0.8910	 0.6440
Y	 0.8400	 0.6090
Z	 0.8650	 0.6110
a	 0.8870	 0.6420
b	 0.8400	 0.6020
c	 0.8590	 0.6140
d	 0.8880	 0.6420
e	 0.8390	 0.6030
f	 0.8670	 0.6100
g	 0.8900	 0.6410
h	 0.8430	 0.6070



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Chain	Atom inclusion	Q-score
i	 0.8590	 0.6110
j	 0.8810	 0.6410
k	 0.8420	 0.6050
l	 0.8670	 0.6110
m	 0.8860	 0.6390