



Full wwPDB EM Validation Report ⓘ

Mar 22, 2024 – 10:12 AM EDT

PDB ID : 9B40
EMDB ID : EMD-44163
Title : Pseudomonas phage Pa193 5-fold vertex (capsid, decorating, and scaffolding proteins)
Deposited on : 2024-03-20
Resolution : 2.90 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

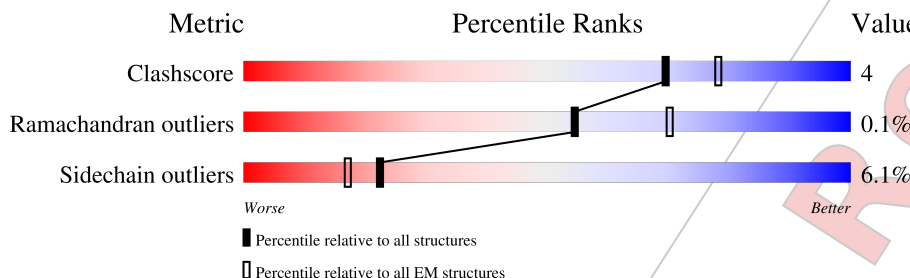
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.90 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.



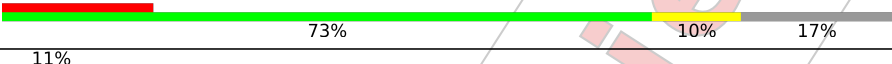
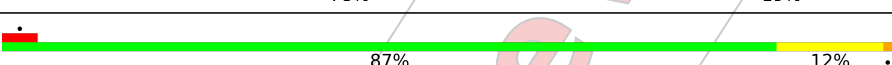
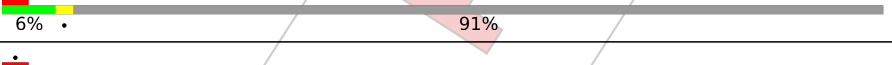
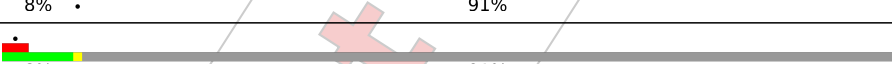
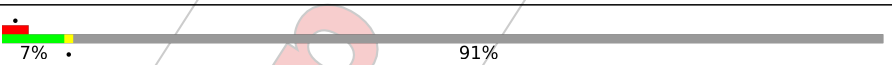
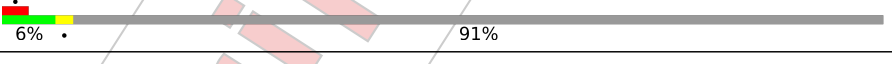
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	382	
1	B	382	
1	C	382	
1	D	382	
1	E	382	
1	N	382	
1	O	382	
1	P	382	

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Mol	Chain	Length	Quality of chain
1	Q	382	
1	R	382	
1	S	382	
2	K	211	
2	L	211	
2	M	211	
3	F	478	
3	G	478	
3	H	478	
3	I	478	
3	J	478	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32946 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 gp26 Major capsid.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	B	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	C	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	D	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	E	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	N	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	O	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	P	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	Q	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	R	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		
1	S	317	Total	C	N	O	S	0	0
			2447	1553	416	472	6		

- Molecule 2 is a protein called gp25 Decorating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	211	Total	C	N	O	S	0	0
			1528	971	262	291	4		
2	L	211	Total	C	N	O	S	0	0
			1528	971	262	291	4		
2	M	211	Total	C	N	O	S	0	0
			1528	971	262	291	4		

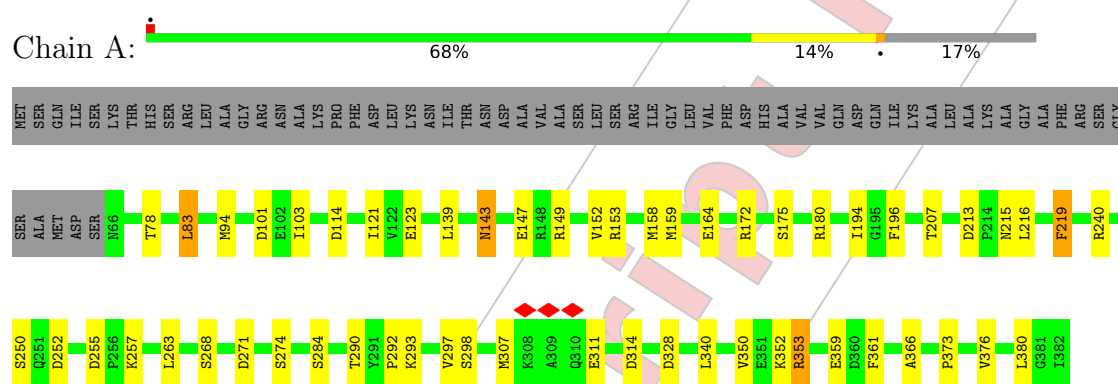
- Molecule 3 is a protein called gp24 Scaffolding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	41	Total	C	N	O	S	0	0
			289	173	50	65	1		
3	F	41	Total	C	N	O	S	0	0
			289	173	50	65	1		
3	H	41	Total	C	N	O	S	0	0
			289	173	50	65	1		
3	I	41	Total	C	N	O	S	0	0
			289	173	50	65	1		
3	J	41	Total	C	N	O	S	0	0
			289	173	50	65	1		

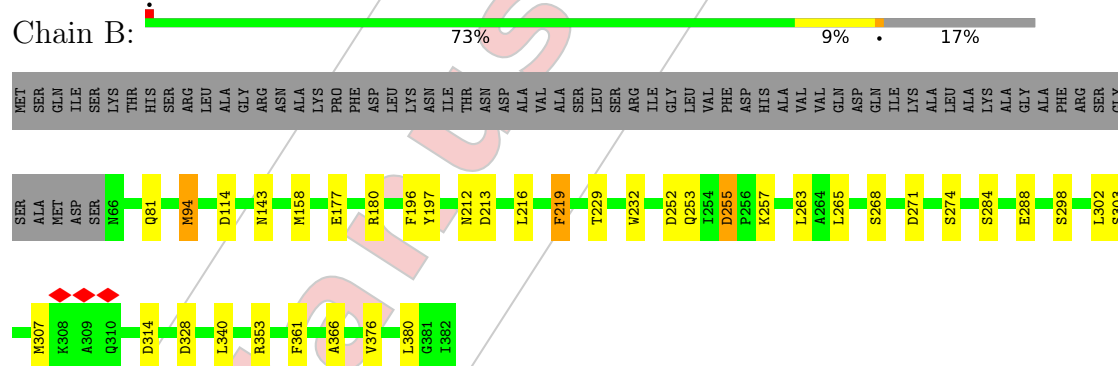
3 Residue-property plots

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

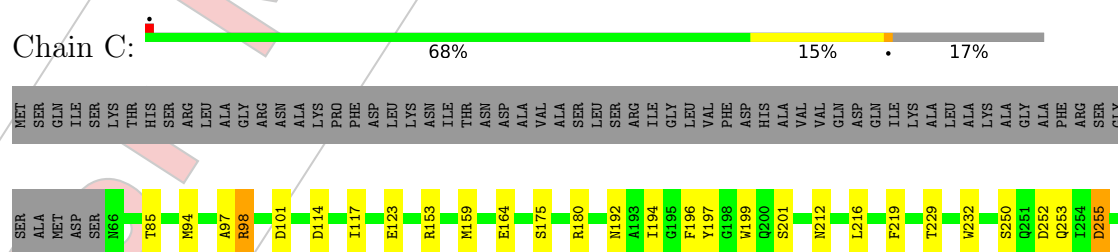
- Molecule 1: gp26 Major capsid



- Molecule 1: gp26 Major capsid

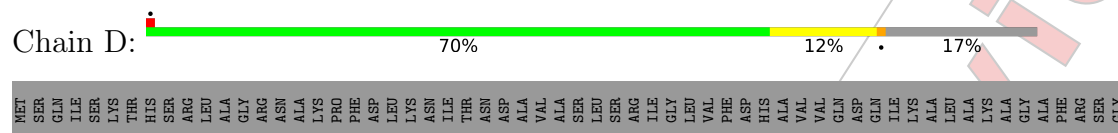


- Molecule 1: gp26 Major capsid

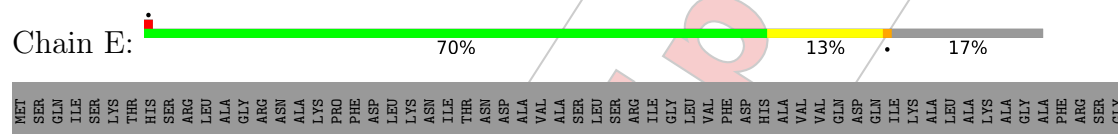




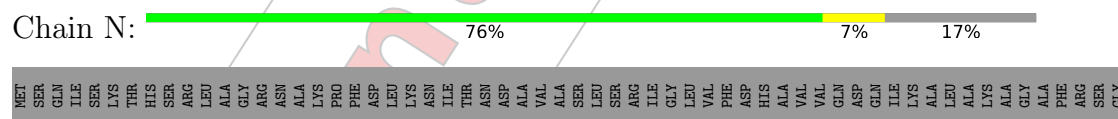
- Molecule 1: gp26 Major capsid



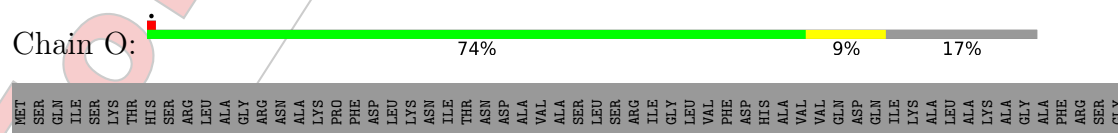
- Molecule 1: gp26 Major capsid

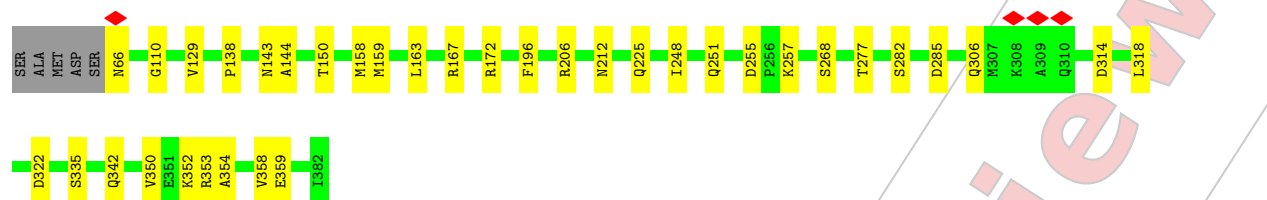


- Molecule 1: gp26 Major capsid



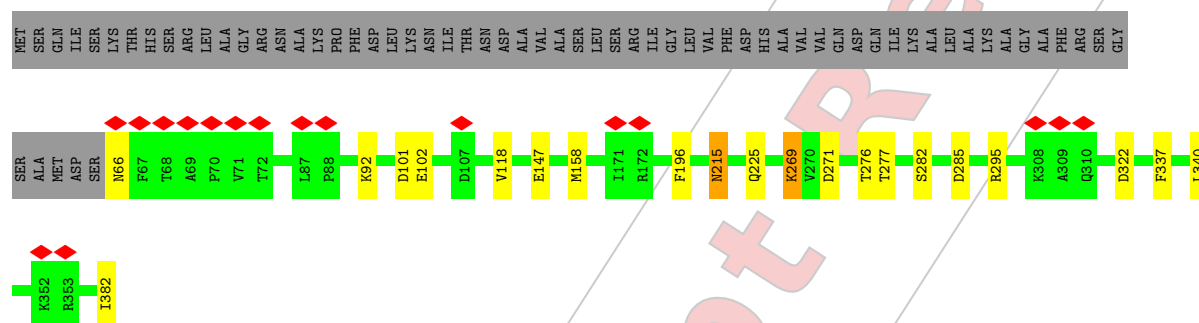
- Molecule 1: gp26 Major capsid





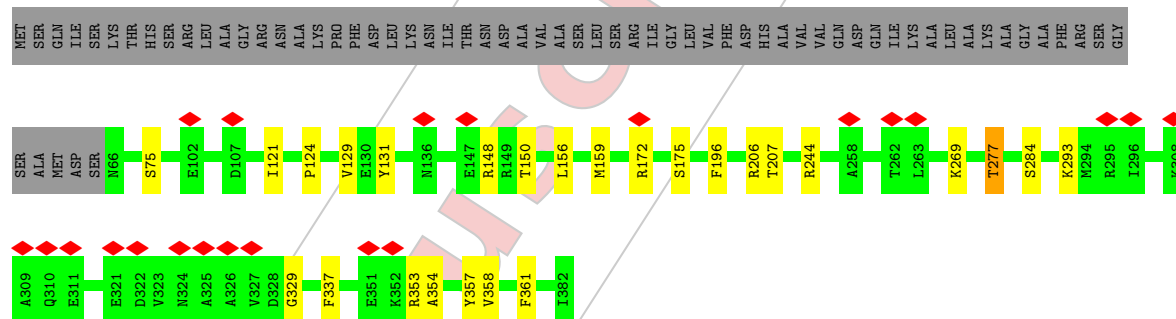
- Molecule 1: gp26 Major capsid

Chain P: 77% 5% 17%



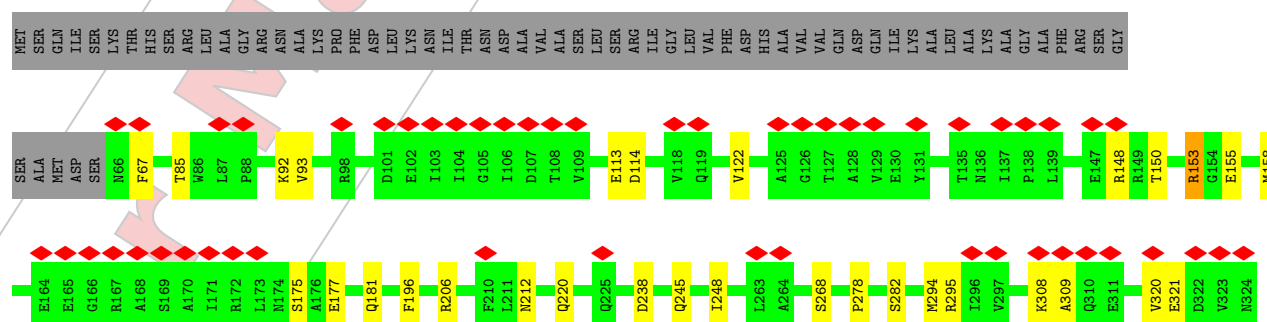
- Molecule 1: gp26 Major capsid

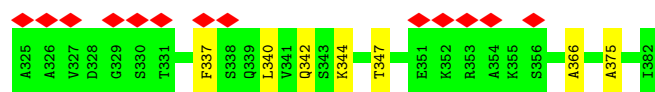
Chain Q: 6% 76% 7% 17%



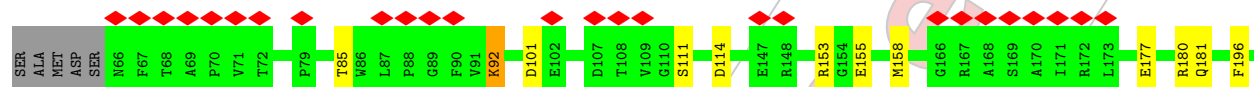
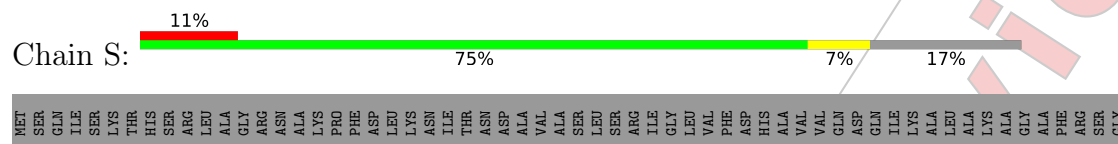
- Molecule 1: gp26 Major capsid

Chain R: 17% 73% 10% 17%

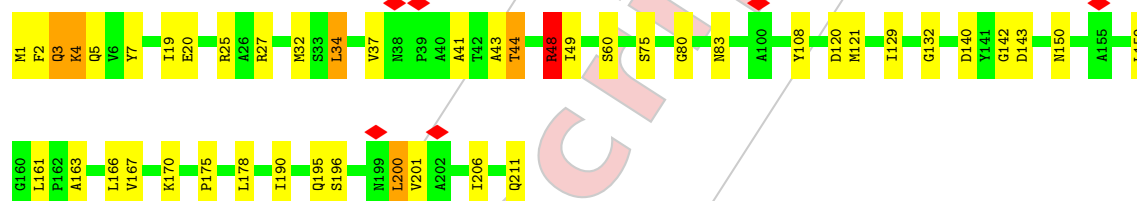
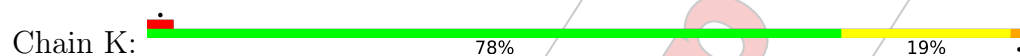




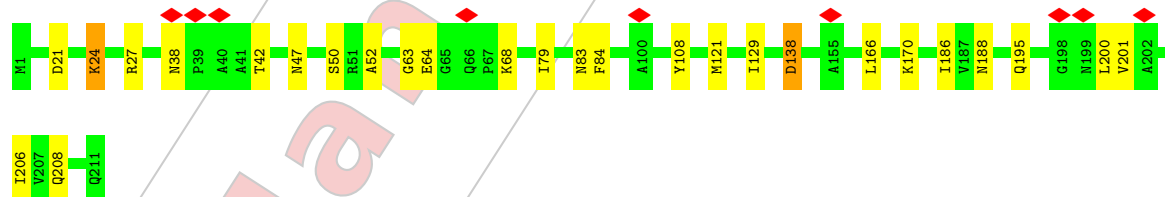
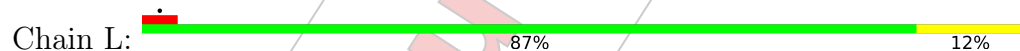
- Molecule 1: gp26 Major capsid



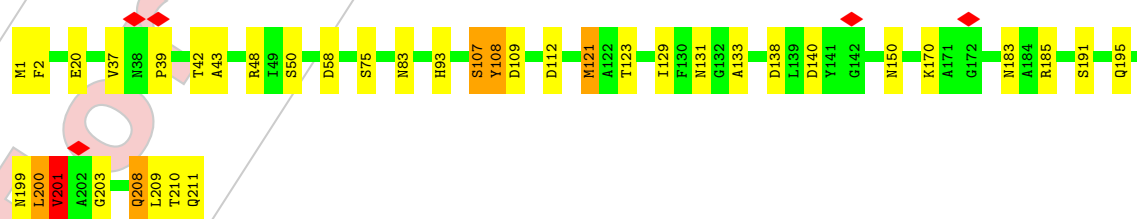
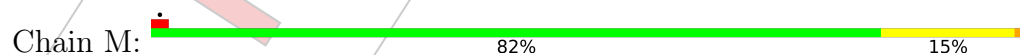
- Molecule 2: gp25 Decorating protein



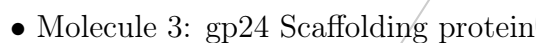
- Molecule 2: gp25 Decorating protein



- Molecule 2: gp25 Decorating protein



Chain G: 8% 91%



Chain F: 6% . 91%



GLU
ALA
LEU
ALA
LEU
ASP
MET
TYR
LEU
LYS
GLY
VAL
GLU
ALA
SER
ARG
GLY
ALA
ALA
SER
ARG
GLN
SER
LYS
ALA
GLN
ASP
SER
ALA
GLY
SER
ALA
PRO
GLN
CYS
ALA
ALA
GLU
LEU
LEU
ASP
SER
TYR
LEU
LYS
GLY
GLU

- Molecule 3: gp24 Scaffolding protein

Chain H: 8% 91%

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

HIS	LEU	SER	PHE	ASP	PHE	ARG	PRO	SER	ASP	GLU	GLY	ASN	GLU	MET	SER	LEU	LYS	LYS	ALA	ALA	LYS	LYS	GLN	GLN	PRO	PRO	VAL	GLN	ARG	VAL	GLY	GLN	ALA	ALA	ASP	SER	ALA	VAL	GLU	GLU	LEU	ARG	ALA	LEU	LEU	TRP	PRO	LYS	LYS	LEU	SER	SER	VAL	GLN	LYS	PHE	LEU	GLY	GLU	GLU	ALA	TYR
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GLU	PRO	GLU	HIS	GLN	GLU	GLY	ALA	ALA	ALA	ALA	ALA	GLU	PRO	THR	ASP	SER	GLU	HIS	MET	THR	GLU	HIS	PRO	PRO	THR	LEU	GLU	GLY	GLN	GLN	ASP	ASN	GLU	HIS	GLU	GLU	GLU	GLU	ALA	PRO	PRO	VAL	VAL	ASP	PRO	A286	V287	A288	A289	A290	E291	S292	E293	R294	E295	E296	S300	E301	M302
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S303
R321
L322
F323
G324
T325
A326
ALA
GLU
GLY
ALA
ASP
GLU
GLU
GLY
HIS
GLY
GLY
GLU
GLY
LYS
ASP
VAL
VAL
GLU
GLY
LEU
GLU
GLU
GLN
SER
SER
SER
GLY
GLN
THR
ALA
ALA
SER
ASP
ASP
GLY
GLY
GLY
LYS
ASP
ASN
SER
GLU
LEU
PRO
GLU
MET
ALA
GLN
LYS
ASN
ALA

[illegible]

ASP	MET	TYR	LEU	LYS	GLY	VAL	GLU	ALA	ALA	SER	ARG	GLY	GLY	ALA	ALA	SER	ARG	GLN	SER	LYS	ALA	GLN	ASP	SER	ALA	GLY	SER	ALA	PRO	GLN	CYS	ALA	GLU	LEU	ASP	SER	TYR	LEU	LYS	GLY	GLU
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- Molecule 3: gp24 Scaffolding protein

Chain I: 

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

[illegible]

GLU	PRO	GLU	GLN	HIS	GLY	ALA	ALA	PRO	ALA	GLU	PRO	THR	ASP	SER	GLU	HIS	MET	THR	GLU	HIS	PRO	THR	LEU	GLU	GLY	ALA	GLN	LYS	ASP	ASN	GLU	GLU	GLU	GLU	ALA	PRO	SER	VAL	VAL	ASP	PRO	A286	V287	A288	A289	A290	E291	E292	E293	R294	Q295	E301	E310
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R321 L322 G323 G324 T325 A326
ALA
GLU
GLY
GLY
ALA
ASP
GLU
GLU
GLY
HIS
GLY
GLY
GLY
LYS
ASP
VAL
VAL
VAL
GLU
GLY
LEU
GLU
GLU
GLN
SER
SER
SER
LEU
GLY
GLY
SER
GLN
THR
ALA
SER
SER
ASP
ASP
GLY
GLY
GLY
GLU
GLY
LYS
LYS
ASP
ASN
SER
SER
GLU
GLU
LEU
PRO
MET
GLU
ALA
GLN
LYS
ASN
ASN
GLN
GLN
SER

ALA	LEU	ASP	MET	TYR	LEU	LYS	GLY	VAL	GLU	ALA	SER	ARG	GLY	ALA	ALA	SER	GLN	SER	LYS	ALA	GLN	ASP	SER	ALA	GLY	SER	ALA	PRO	GLN	CYS	ALA	GLU	LEU	ASP	SER	TYR	LEU	LYS	GLY
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	8278	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)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	27.436	Depositor
Minimum map value	-12.877	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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	0.29	0/2500	0.53	0/3403
1	B	0.28	0/2500	0.53	0/3403
1	C	0.30	0/2500	0.55	0/3403
1	D	0.29	0/2500	0.54	0/3403
1	E	0.29	0/2500	0.54	0/3403
1	N	0.27	0/2500	0.51	0/3403
1	O	0.28	0/2500	0.55	0/3403
1	P	0.27	0/2500	0.52	0/3403
1	Q	0.27	0/2500	0.52	0/3403
1	R	0.27	0/2500	0.54	0/3403
1	S	0.27	0/2500	0.53	0/3403
2	K	0.37	0/1562	0.56	0/2130
2	L	0.30	0/1562	0.54	0/2130
2	M	0.33	0/1562	0.57	0/2130
3	F	0.49	0/288	0.57	0/386
3	G	0.31	0/288	0.54	0/386
3	H	0.30	0/288	0.51	0/386
3	I	0.47	0/288	0.52	0/386
3	J	0.42	0/288	0.50	0/386
All	All	0.29	0/33626	0.54	0/45753

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	K	0	1
3	F	0	2
3	I	0	1
3	J	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	98	ARG	Sidechain
3	F	294	ARG	Sidechain
3	F	299	ALA	Mainchain
3	I	294	ARG	Sidechain
3	J	294	ARG	Sidechain
2	K	48	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2447	0	2421	31	0
1	B	2447	0	2421	18	0
1	C	2447	0	2421	27	0
1	D	2447	0	2421	23	0
1	E	2447	0	2421	26	0
1	N	2447	0	2421	12	0
1	O	2447	0	2421	12	0
1	P	2447	0	2421	11	0
1	Q	2447	0	2421	12	0
1	R	2447	0	2421	19	0
1	S	2447	0	2421	15	0
2	K	1528	0	1514	39	0
2	L	1528	0	1514	14	0
2	M	1528	0	1514	25	0
3	F	289	0	284	3	0
3	G	289	0	284	4	0
3	H	289	0	284	3	0
3	I	289	0	284	3	0
3	J	289	0	284	5	0
All	All	32946	0	32593	241	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 4.

All (241) 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:78:THR:HG21	1:D:83:LEU:HD21	1.53	0.89
1:A:147:GLU:HB2	2:K:1:MET:HG2	1.57	0.87
1:E:78:THR:HG21	1:E:83:LEU:HD21	1.56	0.83
1:R:248:ILE:HD11	1:S:268:SER:HA	1.63	0.81
1:A:78:THR:HB	1:A:83:LEU:HD11	1.66	0.76
2:K:167:VAL:HG21	2:K:178:LEU:HD21	1.67	0.76
2:K:195:GLN:HB3	2:K:201:VAL:HG12	1.69	0.74
2:K:25:ARG:HD3	2:M:123:THR:HG23	1.71	0.73
1:B:257:LYS:NZ	3:H:302:MET:O	2.21	0.71
2:L:195:GLN:HB3	2:L:201:VAL:HG12	1.71	0.71
1:N:268:SER:HA	1:O:248:ILE:HD11	1.74	0.69
3:J:292:SER:HA	3:J:295:GLN:HE21	1.58	0.69
2:K:37:VAL:HG11	2:K:41:ALA:HB2	1.75	0.68
1:S:177:GLU:OE1	1:S:181:GLN:NE2	2.27	0.67
2:K:20:GLU:OE1	2:L:27:ARG:NH1	2.28	0.67
2:L:63:GLY:O	2:L:68:LYS:NZ	2.30	0.64
1:D:253:GLN:NE2	1:E:94:MET:SD	2.71	0.63
3:J:297:SER:O	3:J:301:GLU:HG2	1.99	0.62
1:C:159:MET:HG3	1:C:358:VAL:HG22	1.83	0.61
1:P:118:VAL:HA	1:P:147:GLU:O	2.01	0.61
2:K:27:ARG:NH1	2:M:20:GLU:OE1	2.33	0.60
2:M:138:ASP:O	2:M:170:LYS:NZ	2.32	0.60
1:C:180:ARG:NH1	1:C:359:GLU:OE1	2.34	0.60
1:E:295:ARG:NH1	3:J:301:GLU:OE2	2.35	0.59
1:A:103:ILE:HG12	1:A:297:VAL:HG11	1.85	0.59
1:A:159:MET:SD	1:A:353:ARG:NH2	2.76	0.59
1:C:98:ARG:HB3	1:C:192:ASN:HB2	1.84	0.59
1:R:220:GLN:OE1	1:R:245:GLN:NE2	2.36	0.59
2:M:37:VAL:HG12	2:M:39:PRO:HD2	1.84	0.58
1:C:353:ARG:HH21	1:C:358:VAL:HG21	1.67	0.58
2:K:37:VAL:CG1	2:K:41:ALA:HB2	2.33	0.58
1:P:282:SER:OG	1:P:285:ASP:OD2	2.21	0.58
1:A:180:ARG:NH1	1:A:359:GLU:OE1	2.36	0.57
1:O:143:ASN:OD1	1:O:144:ALA:N	2.37	0.57
1:N:247:ARG:NH2	1:N:255:ASP:OD1	2.37	0.57
1:B:94:MET:HG2	2:K:3:GLN:HE22	1.67	0.57
1:S:313:GLU:HG2	1:S:381:GLY:HA2	1.87	0.57
2:K:43:ALA:HB3	2:K:150:ASN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:131:TYR:HB3	1:R:153:ARG:HG3	1.87	0.57
1:C:164:GLU:OE2	1:C:175:SER:OG	2.23	0.56
1:D:164:GLU:OE2	1:D:175:SER:OG	2.24	0.56
1:A:164:GLU:OE2	1:A:175:SER:OG	2.23	0.56
1:A:340:LEU:HB2	1:A:366:ALA:HB3	1.87	0.56
1:E:197:TYR:O	1:E:212:ASN:ND2	2.38	0.56
1:A:123:GLU:HB3	1:A:143:ASN:HD21	1.70	0.56
1:E:164:GLU:OE2	1:E:175:SER:OG	2.24	0.56
1:Q:244:ARG:NH1	1:R:268:SER:O	2.39	0.55
2:K:190:ILE:HG12	2:K:206:ILE:HD13	1.87	0.55
2:K:83:ASN:ND2	2:M:140:ASP:OD2	2.39	0.54
1:O:268:SER:OG	1:O:314:ASP:OD2	2.24	0.54
2:M:43:ALA:HB3	2:M:150:ASN:HA	1.88	0.54
2:L:138:ASP:O	2:L:170:LYS:NZ	2.40	0.54
1:A:268:SER:OG	1:A:314:ASP:OD2	2.25	0.53
2:K:25:ARG:NH1	2:M:209:LEU:HD11	2.24	0.53
1:R:114:ASP:OD2	1:S:85:THR:OG1	2.26	0.53
1:C:268:SER:OG	1:C:314:ASP:OD2	2.26	0.53
2:M:195:GLN:HB2	2:M:200:LEU:O	2.08	0.53
1:D:340:LEU:HB2	1:D:366:ALA:HB3	1.89	0.53
1:O:282:SER:OG	1:O:285:ASP:OD2	2.21	0.53
1:Q:124:PRO:HD2	1:R:93:VAL:HG22	1.92	0.52
1:A:298:SER:OG	1:E:252:ASP:OD1	2.28	0.52
3:H:296:GLU:O	3:H:300:SER:OG	2.28	0.52
1:D:252:ASP:OD2	1:E:298:SER:OG	2.25	0.52
2:K:25:ARG:HG3	2:K:121:MET:HG2	1.89	0.52
2:K:43:ALA:HB1	2:K:163:ALA:HA	1.90	0.52
1:E:216:LEU:HD22	1:E:376:VAL:HG11	1.92	0.52
2:K:132:GLY:HA3	2:K:175:PRO:CG	2.40	0.52
1:A:219:PHE:CD1	1:A:380:LEU:HB2	2.45	0.52
1:A:216:LEU:HD22	1:A:376:VAL:HG11	1.92	0.51
1:A:293:LYS:NZ	3:G:310:GLU:OE2	2.42	0.51
2:M:201:VAL:HG12	2:M:201:VAL:O	2.09	0.51
1:A:152:VAL:HG23	1:A:207:THR:HG21	1.91	0.51
1:C:216:LEU:HD22	1:C:376:VAL:HG11	1.93	0.51
1:B:253:GLN:NE2	1:C:97:ALA:HB2	2.25	0.51
2:K:5:GLN:HG3	2:K:7:TYR:CZ	2.46	0.51
1:A:123:GLU:HB3	1:A:143:ASN:ND2	2.25	0.51
2:K:132:GLY:HA3	2:K:175:PRO:HG2	1.93	0.51
2:L:64:GLU:N	2:L:64:GLU:OE1	2.44	0.51
1:O:350:VAL:HG22	1:O:359:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:SER:OG	1:E:314:ASP:OD2	2.28	0.51
1:D:219:PHE:CD1	1:D:380:LEU:HB2	2.46	0.50
1:C:197:TYR:O	1:C:212:ASN:ND2	2.42	0.50
1:Q:329:GLY:O	1:R:92:LYS:NZ	2.32	0.50
1:A:139:LEU:N	2:K:19:ILE:O	2.44	0.50
1:B:340:LEU:HB2	1:B:366:ALA:HB3	1.93	0.50
1:N:138:PRO:HG2	1:Q:156:LEU:HA	1.94	0.50
1:A:94:MET:SD	1:E:253:GLN:NE2	2.85	0.49
1:B:232:TRP:CH2	1:C:280:GLY:HA2	2.47	0.49
1:D:268:SER:OG	1:D:314:ASP:OD2	2.30	0.49
1:B:216:LEU:HD22	1:B:376:VAL:HG11	1.94	0.49
1:D:295:ARG:HG3	3:I:301:GLU:HB2	1.94	0.49
1:E:293:LYS:NZ	3:J:310:GLU:OE1	2.45	0.49
1:E:306:GLN:O	1:E:313:GLU:N	2.39	0.49
1:E:340:LEU:HB2	1:E:366:ALA:HB3	1.95	0.49
1:R:122:VAL:HG13	1:S:92:LYS:HB3	1.94	0.49
1:B:219:PHE:CD1	1:B:380:LEU:HB2	2.48	0.49
1:O:150:THR:HG23	1:O:206:ARG:HB2	1.94	0.49
1:R:295:ARG:NH2	1:R:321:GLU:OE2	2.46	0.49
1:D:295:ARG:CG	3:I:301:GLU:HB2	2.43	0.49
2:M:48:ARG:HG3	2:M:108:TYR:HB3	1.95	0.49
2:M:121:MET:HG3	2:M:211:GLN:HB3	1.93	0.48
1:O:159:MET:HG3	1:O:358:VAL:HG22	1.95	0.48
2:M:1:MET:HB2	1:P:215:ASN:HD21	1.78	0.48
1:S:260:LYS:HZ2	1:S:260:LYS:HB3	1.77	0.48
1:C:253:GLN:HG3	1:D:94:MET:SD	2.53	0.48
1:D:232:TRP:CH2	1:E:280:GLY:HA2	2.48	0.48
1:S:268:SER:OG	1:S:314:ASP:OD2	2.27	0.48
2:K:48:ARG:HE	2:K:48:ARG:HB2	1.50	0.48
1:D:216:LEU:HD22	1:D:376:VAL:HG11	1.96	0.48
1:C:340:LEU:HB2	1:C:366:ALA:HB3	1.95	0.48
1:B:268:SER:OG	1:B:314:ASP:OD2	2.31	0.48
2:K:34:LEU:CD2	2:K:41:ALA:HB1	2.44	0.47
2:M:208:GLN:OE1	2:M:210:THR:OG1	2.32	0.47
1:A:271:ASP:O	1:A:274:SER:OG	2.22	0.47
1:N:142:TRP:HE1	1:Q:175:SER:HG	1.62	0.47
1:R:320:VAL:HG12	1:R:375:ALA:HB1	1.95	0.47
3:F:292:SER:O	3:F:295:GLN:HG2	2.14	0.47
1:D:180:ARG:NH1	1:D:359:GLU:OE1	2.46	0.47
1:O:110:GLY:HA3	1:O:342:GLN:HG3	1.97	0.47
1:B:114:ASP:OD2	1:C:85:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:THR:CG2	1:E:83:LEU:HD11	2.44	0.47
1:Q:159:MET:HG3	1:Q:358:VAL:HG22	1.96	0.47
2:K:34:LEU:HD13	2:K:44:THR:HA	1.97	0.47
1:E:78:THR:HG21	1:E:83:LEU:CD2	2.39	0.47
2:K:3:GLN:HA	1:N:71:VAL:HG11	1.97	0.47
1:N:119:GLN:OE1	1:N:120:GLY:N	2.48	0.47
1:A:257:LYS:HD3	1:A:292:PRO:HG2	1.96	0.47
1:C:123:GLU:HG3	1:D:93:VAL:HG21	1.97	0.47
1:O:129:VAL:HG22	1:O:138:PRO:HG3	1.96	0.47
1:Q:353:ARG:HD2	1:Q:354:ALA:H	1.80	0.47
1:B:177:GLU:OE1	1:B:180:ARG:NH1	2.48	0.46
2:K:129:ILE:HA	2:K:166:LEU:O	2.15	0.46
2:M:131:ASN:ND2	2:M:133:ALA:O	2.42	0.46
2:L:50:SER:O	2:L:50:SER:OG	2.32	0.46
1:E:117:ILE:HG21	1:E:340:LEU:HD13	1.97	0.46
2:M:129:ILE:O	2:M:203:GLY:HA3	2.16	0.46
1:A:149:ARG:NH2	1:A:213:ASP:OD1	2.49	0.46
1:C:232:TRP:CH2	1:D:280:GLY:HA2	2.50	0.46
1:E:257:LYS:HZ1	3:G:303:SER:HA	1.80	0.46
1:S:316:LEU:HB2	1:S:382:ILE:HD13	1.98	0.46
2:K:129:ILE:HB	2:K:167:VAL:O	2.16	0.46
1:D:293:LYS:NZ	3:I:310:GLU:OE1	2.49	0.46
1:E:350:VAL:HG22	1:E:359:GLU:HG3	1.98	0.46
2:K:80:GLY:O	2:K:150:ASN:N	2.48	0.45
1:P:271:ASP:OD2	1:S:247:ARG:NE	2.46	0.45
1:C:252:ASP:OD2	1:D:298:SER:OG	2.30	0.45
2:L:52:ALA:HB1	2:L:84:PHE:HE1	1.82	0.45
1:P:102:GLU:N	1:P:102:GLU:OE1	2.49	0.45
1:C:316:LEU:HB2	1:C:382:ILE:HD13	1.99	0.45
1:A:373:PRO:HB2	2:K:4:LYS:HG3	1.99	0.45
1:E:219:PHE:CD1	1:E:380:LEU:HB2	2.52	0.45
2:K:161:LEU:HD23	2:K:200:LEU:HD11	1.98	0.45
2:M:107:SER:OG	2:M:109:ASP:OD2	2.35	0.45
1:Q:353:ARG:HD2	1:Q:354:ALA:N	2.32	0.44
1:R:295:ARG:HG2	1:R:295:ARG:HH11	1.83	0.44
1:C:306:GLN:O	1:C:313:GLU:N	2.42	0.44
1:D:78:THR:CG2	1:D:83:LEU:HD11	2.47	0.44
2:K:200:LEU:HD22	2:K:200:LEU:HA	1.77	0.44
1:R:340:LEU:HB2	1:R:366:ALA:HB3	1.99	0.44
1:A:121:ILE:HB	2:K:2:PHE:HD2	1.83	0.44
1:A:350:VAL:HG22	1:A:359:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:150:THR:O	1:Q:207:THR:OG1	2.31	0.44
1:S:111:SER:OG	1:S:114:ASP:OD1	2.35	0.44
2:K:159:LEU:HB3	2:K:200:LEU:HD21	1.99	0.44
1:R:85:THR:O	1:R:85:THR:OG1	2.35	0.44
1:R:150:THR:HG23	1:R:206:ARG:HB2	1.99	0.44
1:B:197:TYR:O	1:B:212:ASN:ND2	2.51	0.44
1:O:353:ARG:HG3	1:O:354:ALA:H	1.82	0.44
1:C:194:ILE:HD12	1:C:199:TRP:HB2	1.99	0.44
2:K:142:GLY:H	2:L:83:ASN:HD21	1.65	0.44
3:F:315:VAL:O	3:F:319:LEU:HD12	2.17	0.44
2:K:48:ARG:HG3	2:K:49:ILE:N	2.33	0.44
1:B:255:ASP:OD1	1:B:255:ASP:N	2.50	0.44
1:C:350:VAL:HG22	1:C:359:GLU:HG3	2.00	0.44
1:D:306:GLN:O	1:D:313:GLU:N	2.40	0.44
1:D:350:VAL:HG22	1:D:359:GLU:HG3	2.00	0.44
2:M:150:ASN:OD1	2:M:150:ASN:N	2.50	0.44
2:M:200:LEU:HB3	2:M:201:VAL:H	1.67	0.44
1:C:271:ASP:O	1:C:274:SER:OG	2.22	0.43
2:K:120:ASP:OD2	2:M:185:ARG:NH2	2.52	0.43
2:L:47:ASN:HA	2:L:79:ILE:HD12	1.99	0.43
1:R:342:GLN:N	1:R:342:GLN:OE1	2.51	0.43
2:M:200:LEU:O	2:M:201:VAL:HG23	2.18	0.43
1:N:328:ASP:OD2	1:N:372:ARG:NH2	2.46	0.43
1:A:328:ASP:OD1	1:A:328:ASP:N	2.49	0.43
1:B:81:GLN:HG3	1:N:81:GLN:HB2	1.99	0.43
1:D:95:THR:O	1:D:96:ALA:C	2.57	0.43
2:M:195:GLN:HE21	2:M:200:LEU:C	2.22	0.43
1:P:92:LYS:N	1:S:330:SER:OG	2.51	0.43
1:A:240:ARG:HG3	1:B:274:SER:OG	2.19	0.43
2:K:34:LEU:HD23	2:K:41:ALA:HB1	2.01	0.43
1:A:290:THR:HG21	1:B:274:SER:HB2	2.01	0.42
2:M:2:PHE:CZ	1:P:147:GLU:HG3	2.54	0.42
1:E:353:ARG:HH21	1:E:358:VAL:HG21	1.83	0.42
2:L:129:ILE:HG22	2:L:166:LEU:HB3	2.02	0.42
2:K:167:VAL:CG2	2:K:178:LEU:HD21	2.42	0.42
2:M:83:ASN:OD1	2:M:83:ASN:N	2.39	0.42
1:S:177:GLU:OE2	1:S:180:ARG:NH1	2.52	0.42
1:E:131:TYR:HE2	1:N:163:LEU:HB2	1.84	0.42
1:A:252:ASP:OD1	1:B:298:SER:OG	2.38	0.42
1:A:292:PRO:O	3:G:303:SER:OG	2.37	0.42
1:E:180:ARG:NH1	1:E:359:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:102:GLU:O	1:P:295:ARG:NH1	2.53	0.42
3:J:298:ALA:O	3:J:302:MET:HG3	2.19	0.42
1:C:255:ASP:HB3	1:C:259:GLU:HB3	2.02	0.42
1:E:257:LYS:HZ2	1:E:257:LYS:HG2	1.69	0.42
1:P:276:THR:OG1	1:P:282:SER:HB3	2.20	0.42
1:C:336:VAL:HG22	1:C:372:ARG:HB2	2.02	0.42
1:N:103:ILE:HG22	1:N:104:ILE:HG23	2.01	0.42
1:D:194:ILE:HG13	1:D:199:TRP:HB2	2.02	0.41
1:R:308:LYS:HG3	1:R:309:ALA:H	1.84	0.41
1:S:260:LYS:HB3	1:S:260:LYS:NZ	2.33	0.41
1:B:252:ASP:OD2	1:C:298:SER:OG	2.30	0.41
1:C:260:LYS:HE3	1:C:260:LYS:HB3	1.68	0.41
2:K:206:ILE:HD12	2:K:206:ILE:HA	1.93	0.41
1:R:177:GLU:O	1:R:181:GLN:HG2	2.20	0.41
2:L:188:ASN:HB3	2:L:206:ILE:HG13	2.02	0.41
1:O:163:LEU:HD21	1:O:167:ARG:HD2	2.01	0.41
1:N:213:ASP:HB3	1:N:216:LEU:HG	2.01	0.41
1:P:269:LYS:HG3	1:P:382:ILE:HD12	2.02	0.41
1:S:306:GLN:HB2	1:S:380:LEU:HD21	2.01	0.41
2:L:186:ILE:HG23	2:L:206:ILE:HD11	2.02	0.41
1:B:328:ASP:OD1	1:B:328:ASP:N	2.52	0.41
1:A:215:ASN:HA	2:K:4:LYS:HE2	2.03	0.41
2:L:129:ILE:HD11	2:L:206:ILE:HD13	2.02	0.41
1:D:264:ALA:HA	1:D:297:VAL:HG23	2.03	0.41
1:N:177:GLU:OE2	1:N:180:ARG:NH1	2.53	0.41
1:A:78:THR:CB	1:A:83:LEU:HD11	2.44	0.41
2:M:199:ASN:O	2:M:200:LEU:C	2.60	0.41
2:M:93:HIS:CD2	1:O:163:LEU:HD22	2.56	0.40
1:Q:277:THR:HG21	1:R:278:PRO:HA	2.03	0.40
1:A:114:ASP:O	1:A:153:ARG:NH1	2.53	0.40
2:L:24:LYS:HA	2:L:121:MET:HG2	2.03	0.40
1:E:247:ARG:HG3	1:E:254:ILE:HD12	2.03	0.40
1:P:276:THR:HG22	1:S:232:TRP:HH2	1.85	0.40
1:Q:129:VAL:O	1:R:155:GLU:N	2.54	0.40
1:C:114:ASP:O	1:C:153:ARG:NH1	2.53	0.40
1:C:292:PRO:O	3:H:303:SER:OG	2.38	0.40
1:E:194:ILE:HG13	1:E:199:TRP:HB2	2.04	0.40
2:K:44:THR:C	2:K:163:ALA:HB2	2.42	0.40
3:G:316:LYS:HE3	3:F:314:GLN:HB3	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	315/382 (82%)	297 (94%)	18 (6%)	0	100	100
1	B	315/382 (82%)	298 (95%)	17 (5%)	0	100	100
1	C	315/382 (82%)	297 (94%)	18 (6%)	0	100	100
1	D	315/382 (82%)	300 (95%)	13 (4%)	2 (1%)	25	58
1	E	315/382 (82%)	299 (95%)	16 (5%)	0	100	100
1	N	315/382 (82%)	306 (97%)	9 (3%)	0	100	100
1	O	315/382 (82%)	308 (98%)	7 (2%)	0	100	100
1	P	315/382 (82%)	308 (98%)	7 (2%)	0	100	100
1	Q	315/382 (82%)	306 (97%)	9 (3%)	0	100	100
1	R	315/382 (82%)	304 (96%)	11 (4%)	0	100	100
1	S	315/382 (82%)	307 (98%)	8 (2%)	0	100	100
2	K	209/211 (99%)	194 (93%)	15 (7%)	0	100	100
2	L	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
2	M	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	29	61
3	F	39/478 (8%)	38 (97%)	0	1 (3%)	5	20
3	G	39/478 (8%)	38 (97%)	1 (3%)	0	100	100
3	H	39/478 (8%)	39 (100%)	0	0	100	100
3	I	39/478 (8%)	38 (97%)	1 (3%)	0	100	100
3	J	39/478 (8%)	39 (100%)	0	0	100	100
All	All	4287/7225 (59%)	4107 (96%)	176 (4%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	201	VAL
1	D	96	ALA

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Mol	Chain	Res	Type
3	F	303	SER
1	D	278	PRO

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	261/312 (84%)	244 (94%)	17 (6%)	17	45
1	B	261/312 (84%)	243 (93%)	18 (7%)	15	41
1	C	261/312 (84%)	242 (93%)	19 (7%)	14	38
1	D	261/312 (84%)	243 (93%)	18 (7%)	15	41
1	E	261/312 (84%)	244 (94%)	17 (6%)	17	45
1	N	261/312 (84%)	251 (96%)	10 (4%)	33	67
1	O	261/312 (84%)	246 (94%)	15 (6%)	20	51
1	P	261/312 (84%)	250 (96%)	11 (4%)	30	63
1	Q	261/312 (84%)	248 (95%)	13 (5%)	24	57
1	R	261/312 (84%)	247 (95%)	14 (5%)	22	54
1	S	261/312 (84%)	250 (96%)	11 (4%)	30	63
2	K	153/153 (100%)	138 (90%)	15 (10%)	8	24
2	L	153/153 (100%)	145 (95%)	8 (5%)	23	55
2	M	153/153 (100%)	140 (92%)	13 (8%)	10	31
3	F	28/381 (7%)	25 (89%)	3 (11%)	6	20
3	G	28/381 (7%)	26 (93%)	2 (7%)	14	40
3	H	28/381 (7%)	28 (100%)	0	100	100
3	I	28/381 (7%)	24 (86%)	4 (14%)	3	10
3	J	28/381 (7%)	25 (89%)	3 (11%)	6	20
All	All	3470/5796 (60%)	3259 (94%)	211 (6%)	22	48

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	101	ASP
1	A	143	ASN
1	A	158	MET
1	A	172	ARG
1	A	194	ILE
1	A	196	PHE
1	A	219	PHE
1	A	250	SER
1	A	255	ASP
1	A	263	LEU
1	A	284	SER
1	A	307	MET
1	A	311	GLU
1	A	352	LYS
1	A	353	ARG
1	A	361	PHE
1	B	94	MET
1	B	143	ASN
1	B	158	MET
1	B	196	PHE
1	B	213	ASP
1	B	219	PHE
1	B	229	THR
1	B	255	ASP
1	B	263	LEU
1	B	265	LEU
1	B	271	ASP
1	B	284	SER
1	B	288	GLU
1	B	302	LEU
1	B	303	SER
1	B	307	MET
1	B	353	ARG
1	B	361	PHE
1	C	94	MET
1	C	98	ARG
1	C	101	ASP
1	C	117	ILE
1	C	196	PHE
1	C	201	SER
1	C	219	PHE
1	C	229	THR

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Mol	Chain	Res	Type
1	C	250	SER
1	C	255	ASP
1	C	276	THR
1	C	277	THR
1	C	284	SER
1	C	302	LEU
1	C	303	SER
1	C	310	GLN
1	C	311	GLU
1	C	361	PHE
1	C	365	THR
1	D	83	LEU
1	D	92	LYS
1	D	94	MET
1	D	101	ASP
1	D	117	ILE
1	D	172	ARG
1	D	196	PHE
1	D	201	SER
1	D	219	PHE
1	D	229	THR
1	D	255	ASP
1	D	277	THR
1	D	284	SER
1	D	303	SER
1	D	311	GLU
1	D	331	THR
1	D	344	LYS
1	D	361	PHE
1	E	83	LEU
1	E	98	ARG
1	E	127	THR
1	E	143	ASN
1	E	172	ARG
1	E	196	PHE
1	E	201	SER
1	E	207	THR
1	E	219	PHE
1	E	229	THR
1	E	277	THR
1	E	284	SER
1	E	302	LEU

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Mol	Chain	Res	Type
1	E	310	GLN
1	E	311	GLU
1	E	331	THR
1	E	351	GLU
2	K	3	GLN
2	K	4	LYS
2	K	32	MET
2	K	34	LEU
2	K	44	THR
2	K	48	ARG
2	K	60	SER
2	K	75	SER
2	K	108	TYR
2	K	140	ASP
2	K	143	ASP
2	K	170	LYS
2	K	196	SER
2	K	200	LEU
2	K	211	GLN
2	L	21	ASP
2	L	24	LYS
2	L	38	ASN
2	L	42	THR
2	L	108	TYR
2	L	138	ASP
2	L	200	LEU
2	L	208	GLN
2	M	42	THR
2	M	50	SER
2	M	58	ASP
2	M	75	SER
2	M	107	SER
2	M	108	TYR
2	M	112	ASP
2	M	121	MET
2	M	183	ASN
2	M	191	SER
2	M	200	LEU
2	M	201	VAL
2	M	208	GLN
1	N	121	ILE
1	N	158	MET

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Mol	Chain	Res	Type
1	N	167	ARG
1	N	252	ASP
1	N	322	ASP
1	N	324	ASN
1	N	337	PHE
1	N	340	LEU
1	N	344	LYS
1	N	361	PHE
1	O	66	ASN
1	O	158	MET
1	O	172	ARG
1	O	196	PHE
1	O	212	ASN
1	O	225	GLN
1	O	251	GLN
1	O	255	ASP
1	O	257	LYS
1	O	277	THR
1	O	306	GLN
1	O	318	LEU
1	O	322	ASP
1	O	335	SER
1	O	352	LYS
1	P	66	ASN
1	P	101	ASP
1	P	158	MET
1	P	196	PHE
1	P	215	ASN
1	P	225	GLN
1	P	269	LYS
1	P	277	THR
1	P	322	ASP
1	P	337	PHE
1	P	340	LEU
1	Q	75	SER
1	Q	121	ILE
1	Q	148	ARG
1	Q	172	ARG
1	Q	196	PHE
1	Q	206	ARG
1	Q	269	LYS
1	Q	277	THR

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Mol	Chain	Res	Type
1	Q	284	SER
1	Q	293	LYS
1	Q	337	PHE
1	Q	357	TYR
1	Q	361	PHE
1	R	67	PHE
1	R	113	GLU
1	R	148	ARG
1	R	153	ARG
1	R	158	MET
1	R	175	SER
1	R	196	PHE
1	R	212	ASN
1	R	238	ASP
1	R	282	SER
1	R	294	MET
1	R	337	PHE
1	R	344	LYS
1	R	347	THR
1	S	92	LYS
1	S	101	ASP
1	S	153	ARG
1	S	155	GLU
1	S	158	MET
1	S	196	PHE
1	S	228	SER
1	S	253	GLN
1	S	327	VAL
1	S	337	PHE
1	S	344	LYS
3	G	302	MET
3	G	313	SER
3	F	294	ARG
3	F	302	MET
3	F	313	SER
3	I	287	VAL
3	I	291	GLU
3	I	295	GLN
3	I	301	GLU
3	J	287	VAL
3	J	294	ARG
3	J	296	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	B	253	GLN
1	B	310	GLN
2	K	3	GLN
2	L	66	GLN
2	M	195	GLN
3	J	295	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 monosaccharides 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.

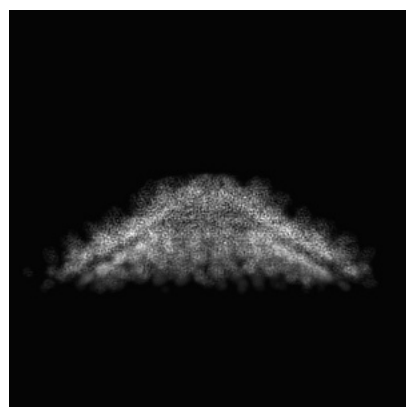
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44163. These allow visual inspection of the internal detail of the map and identification of artifacts.

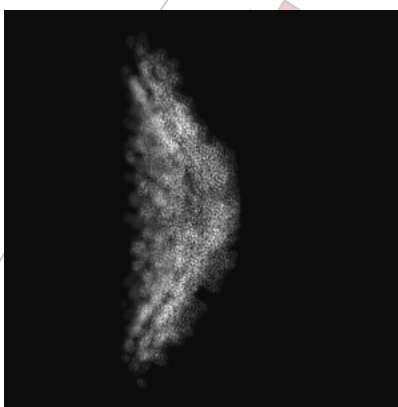
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

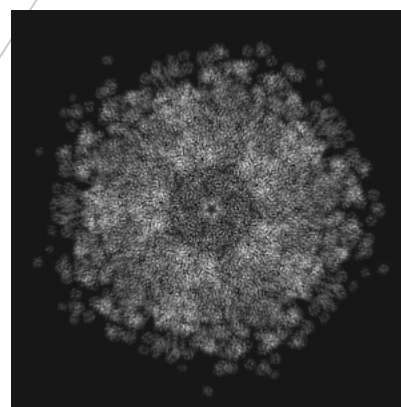
6.1.1 Primary map



X

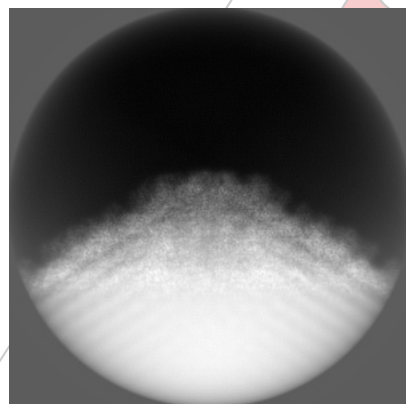


Y

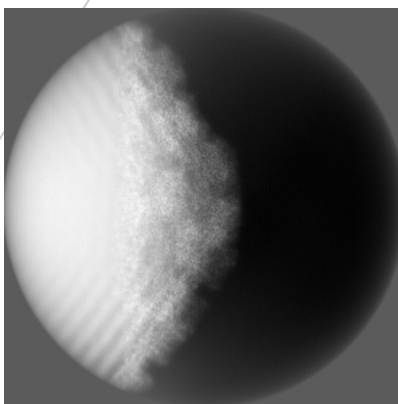


Z

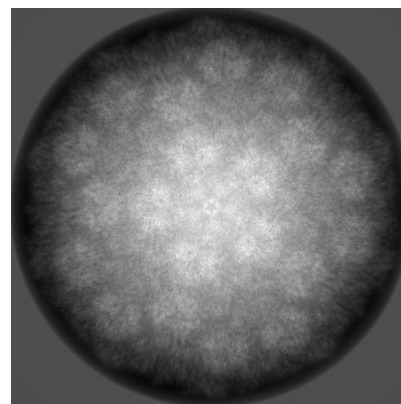
6.1.2 Raw map



X



Y

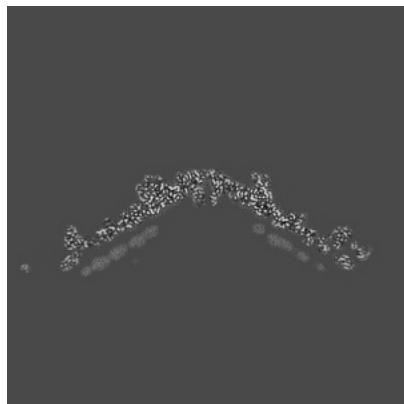


Z

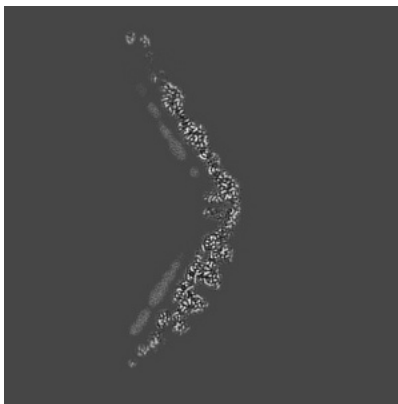
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

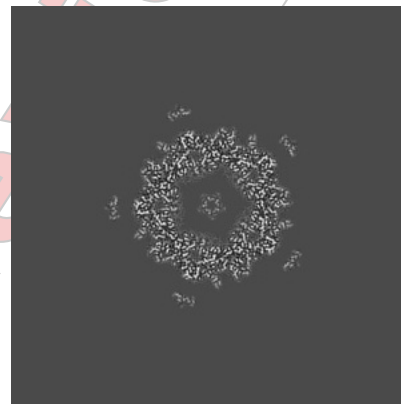
6.2.1 Primary map



X Index: 192

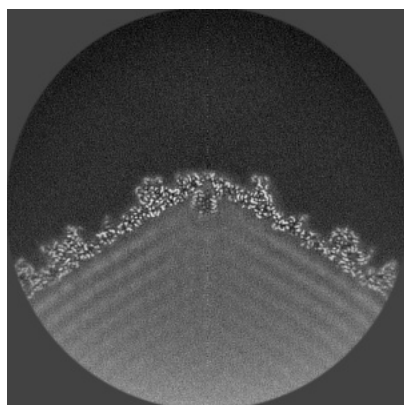


Y Index: 192

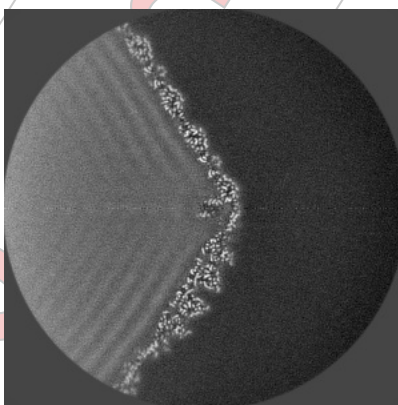


Z Index: 192

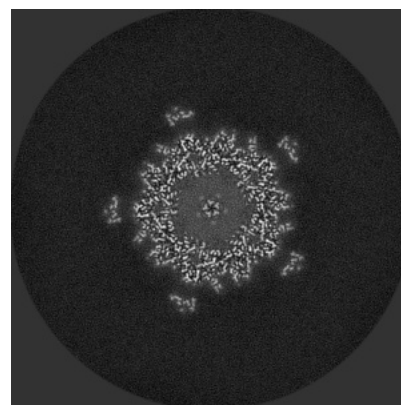
6.2.2 Raw map



X Index: 192



Y Index: 192

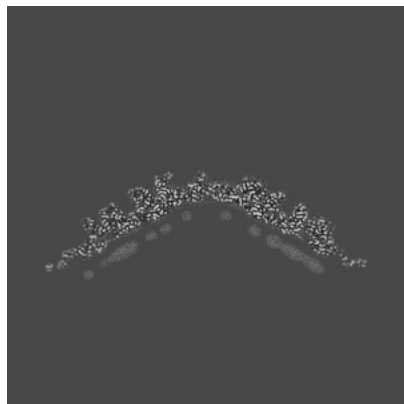


Z Index: 192

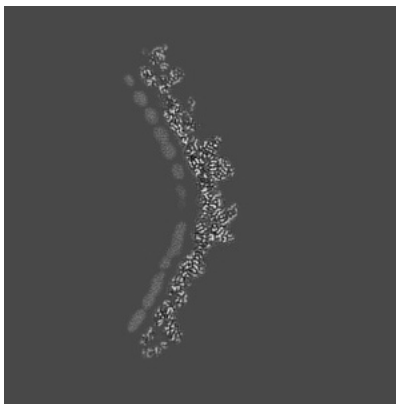
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

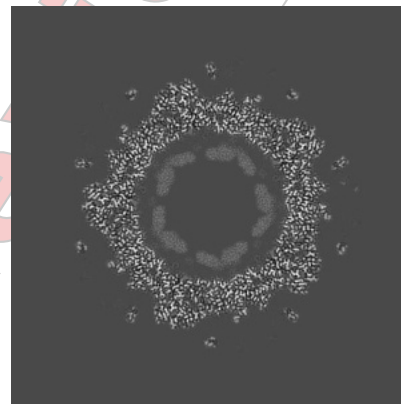
6.3.1 Primary map



X Index: 166

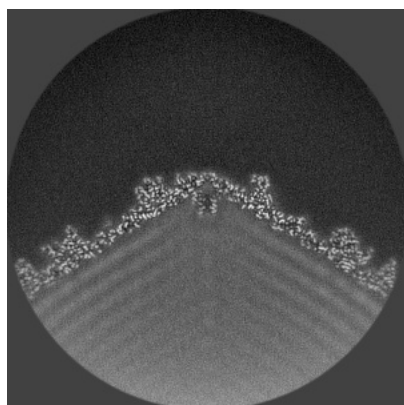


Y Index: 235

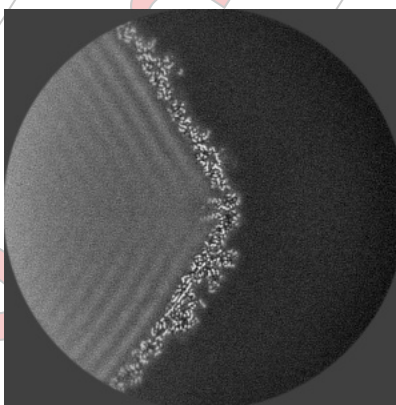


Z Index: 169

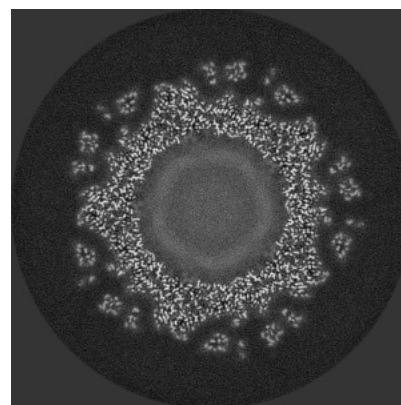
6.3.2 Raw map



X Index: 191



Y Index: 202

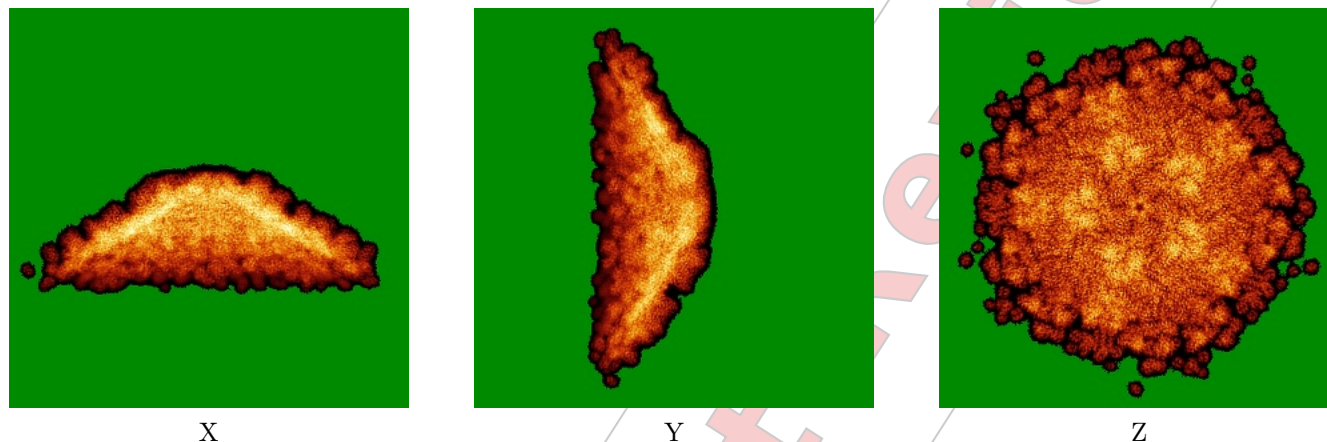


Z Index: 169

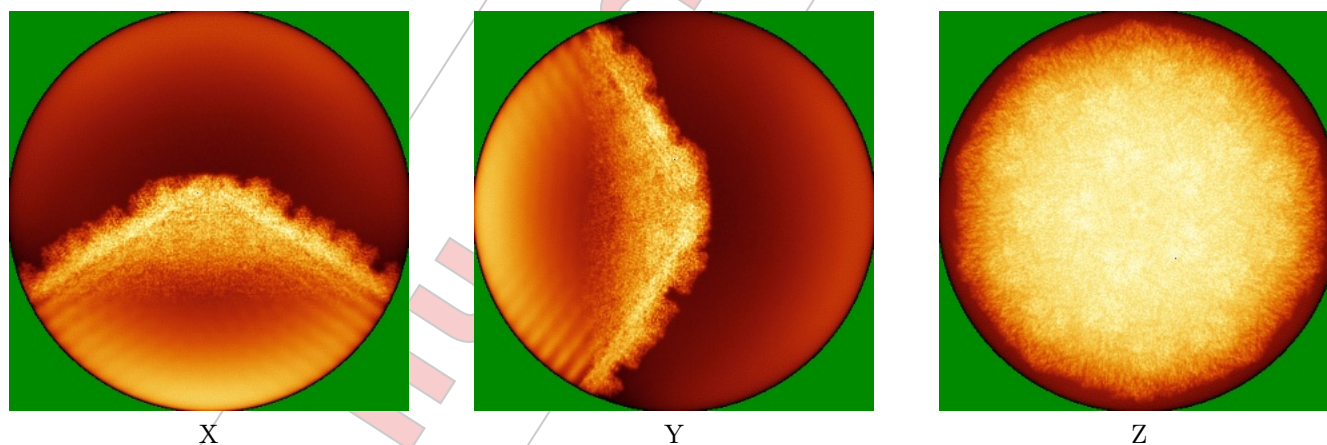
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



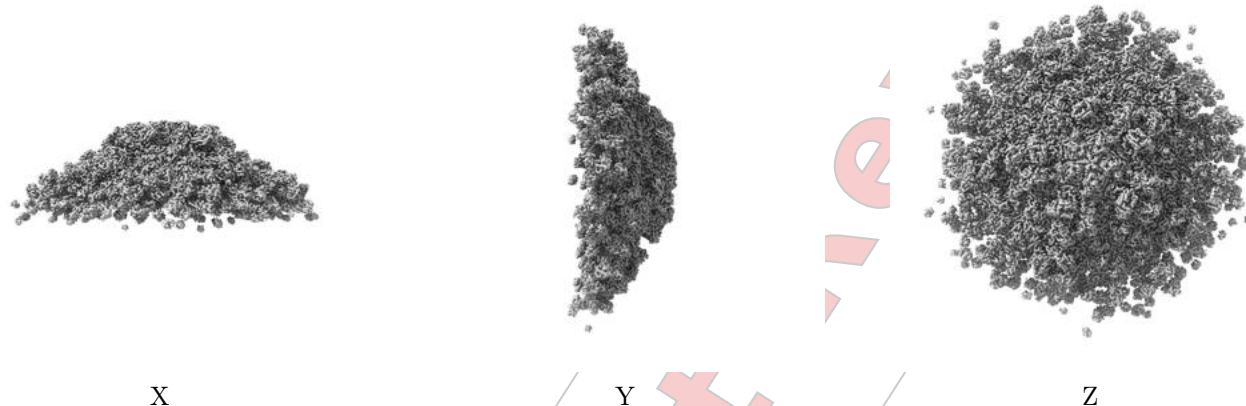
6.4.2 Raw map



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.

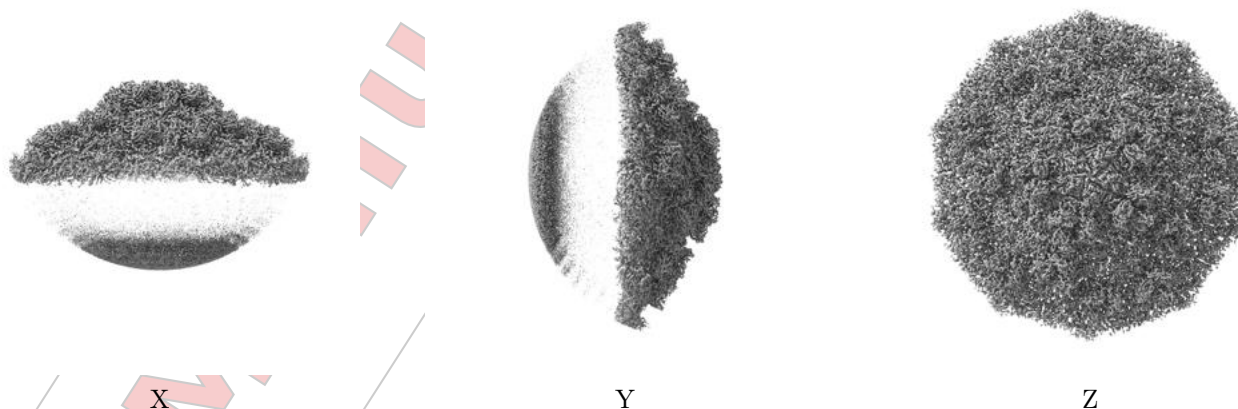
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

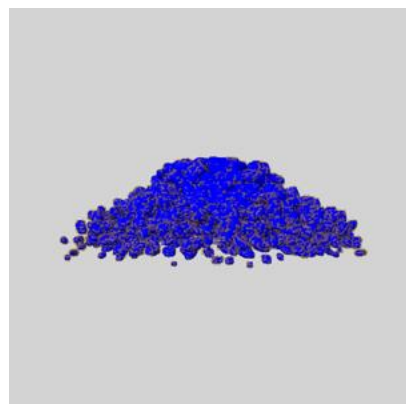
6.6 Mask visualisation [i](#)

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

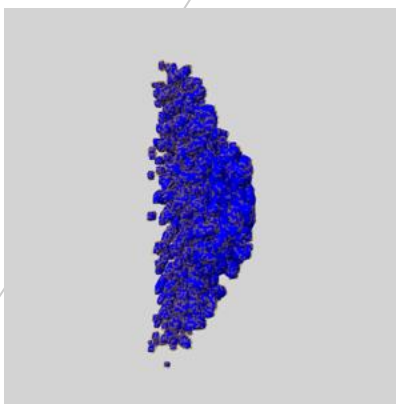
A mask typically either:

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

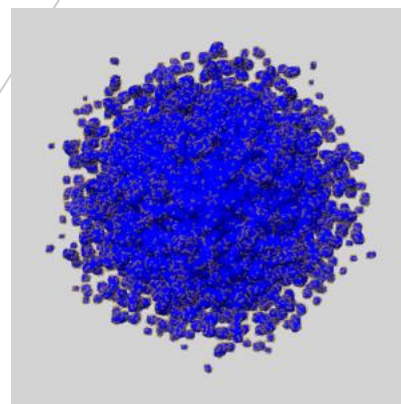
6.6.1 D_1000282537_em-mask-volume_P1.map.V2 [i](#)



X



Y

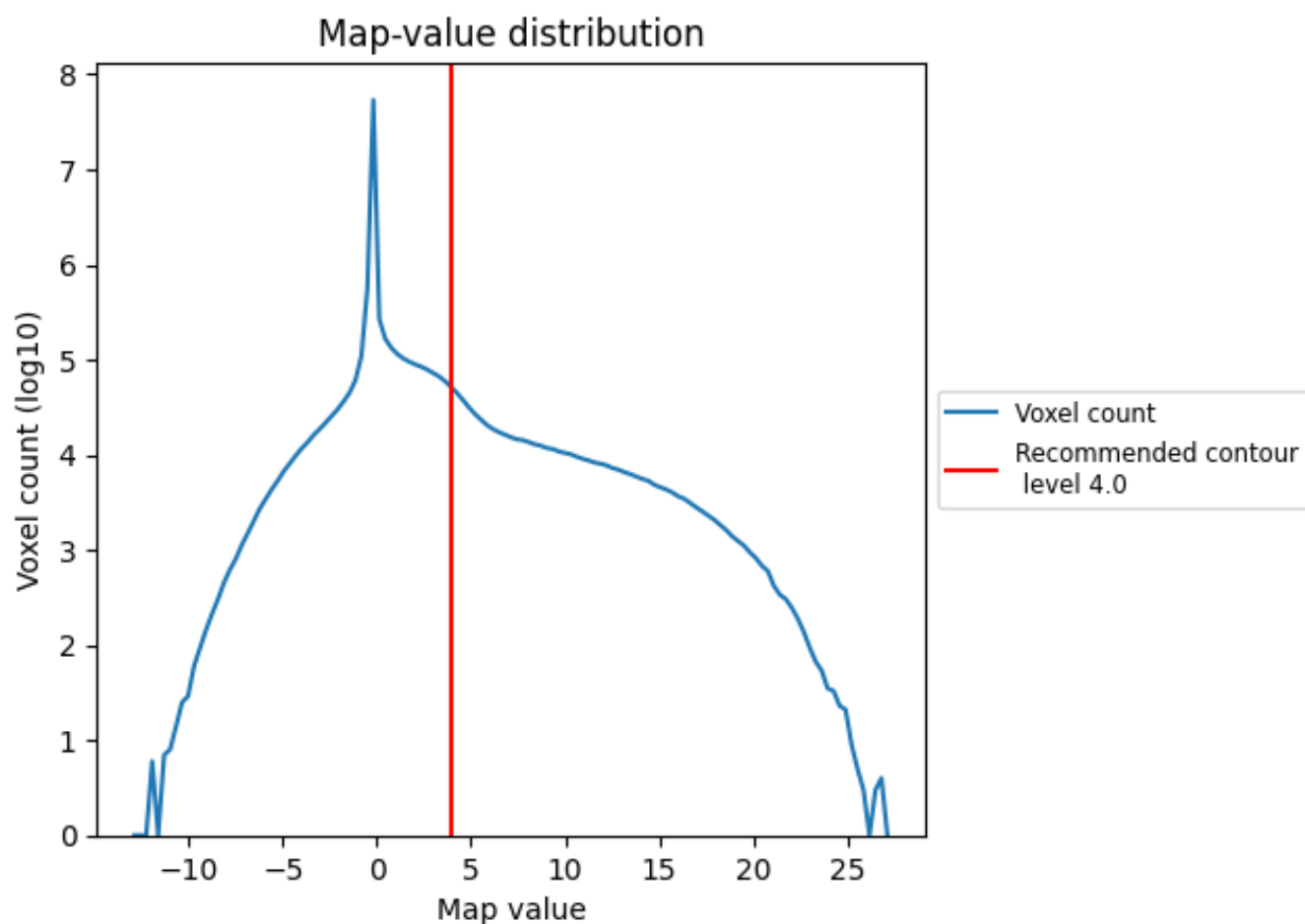


Z

7 Map analysis [i](#)

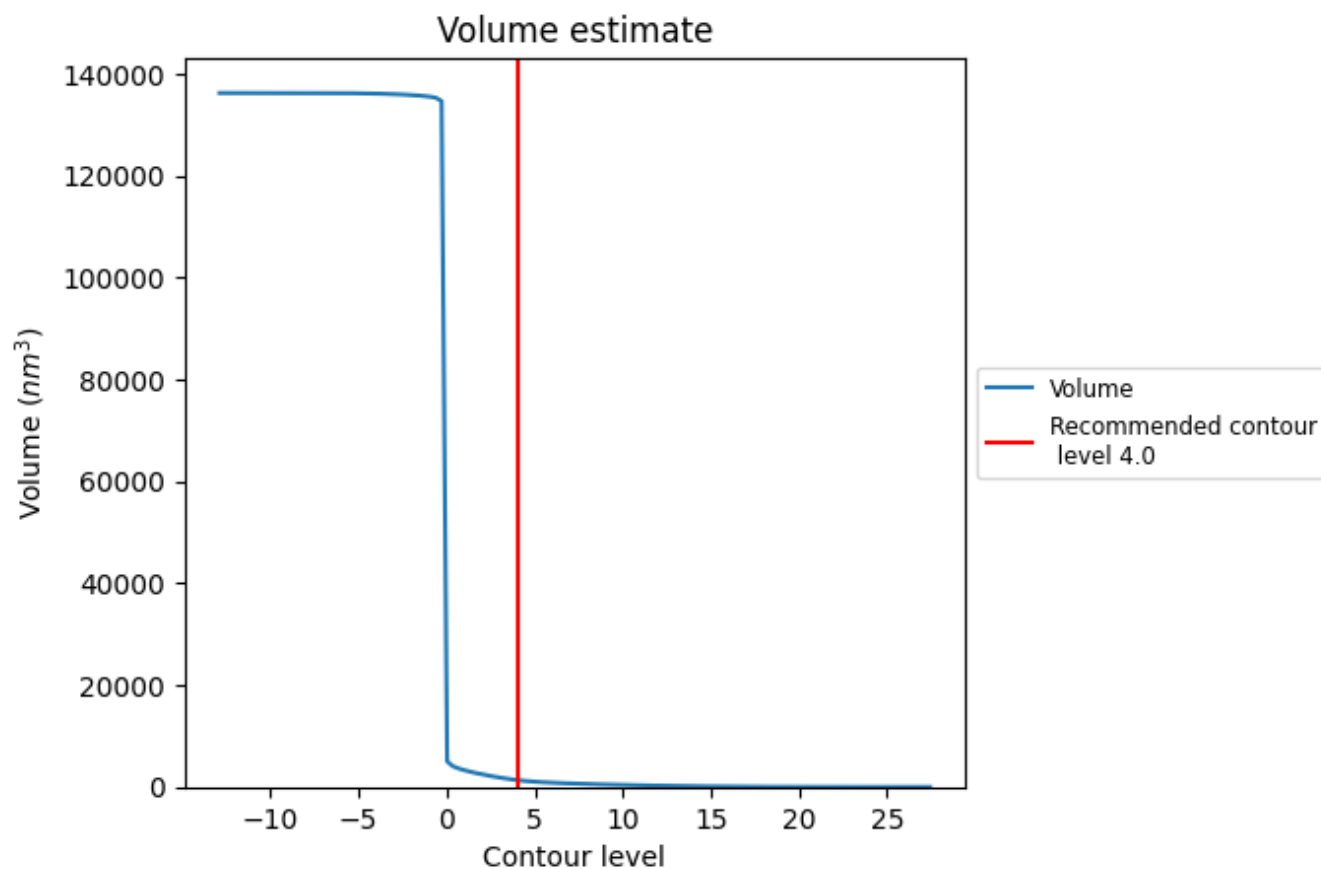
This section contains the results of statistical analysis of the map.

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.

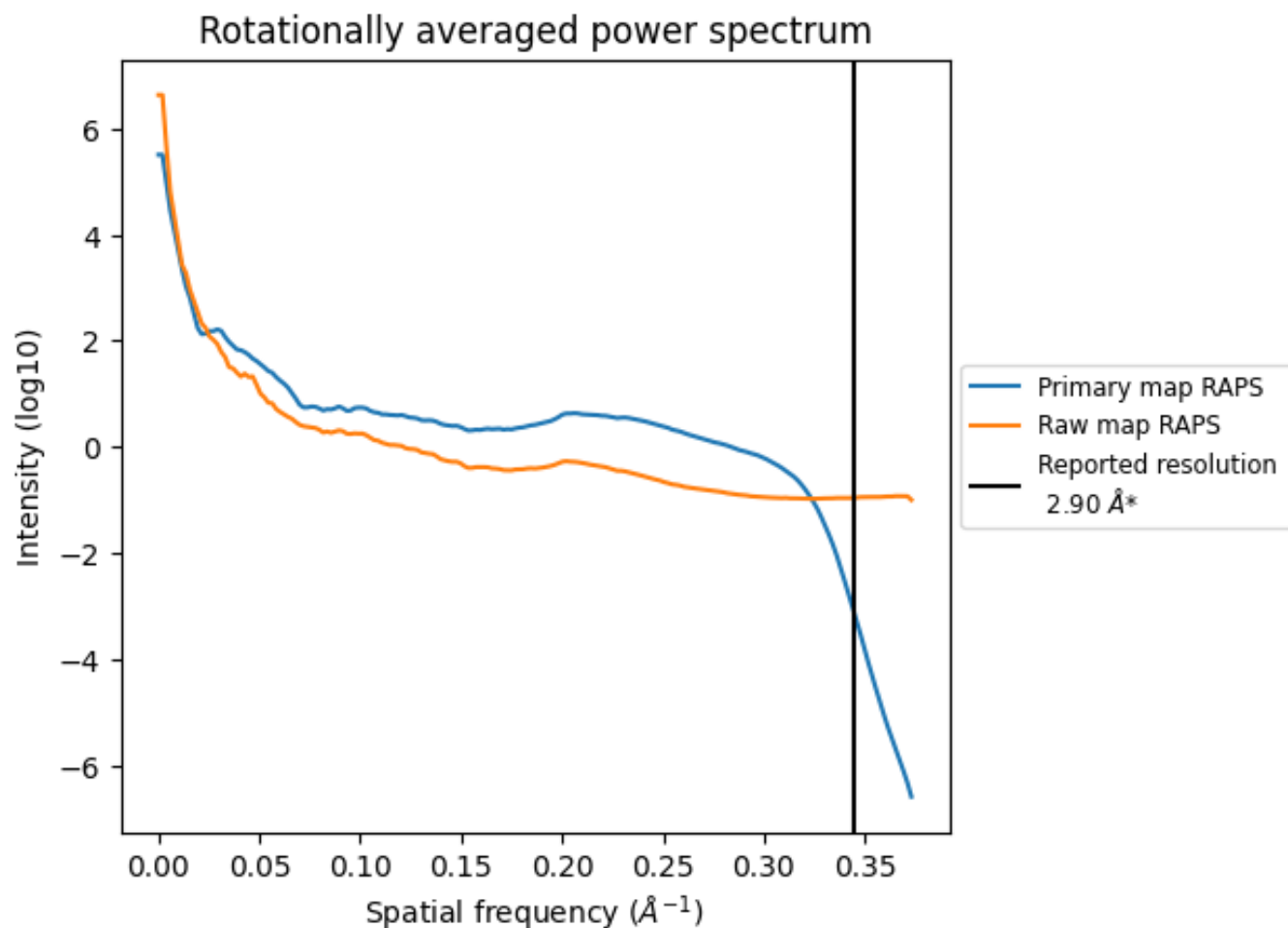
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1356 nm^3 ; this corresponds to an approximate mass of 1225 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 ⓘ

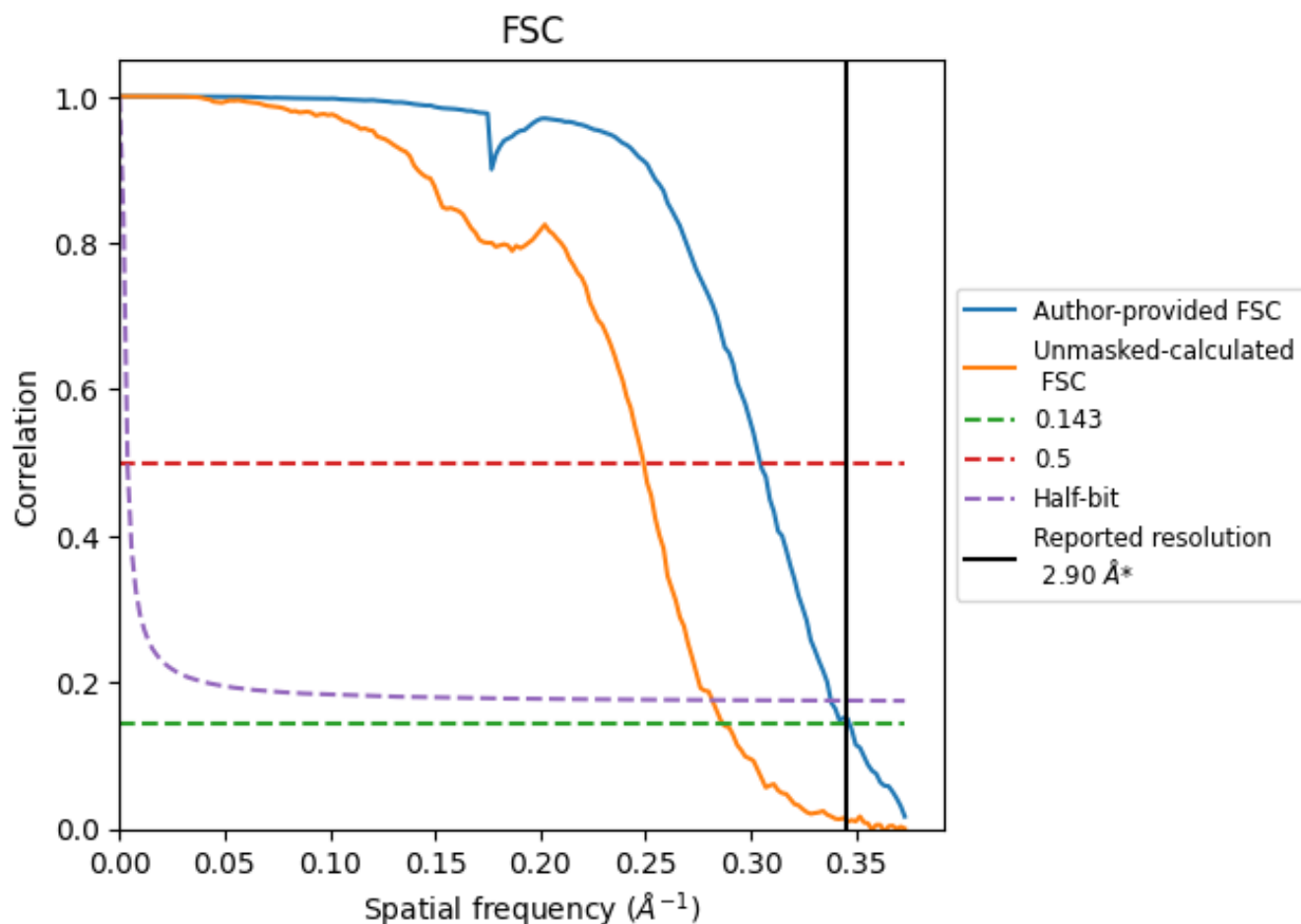


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates ⓘ

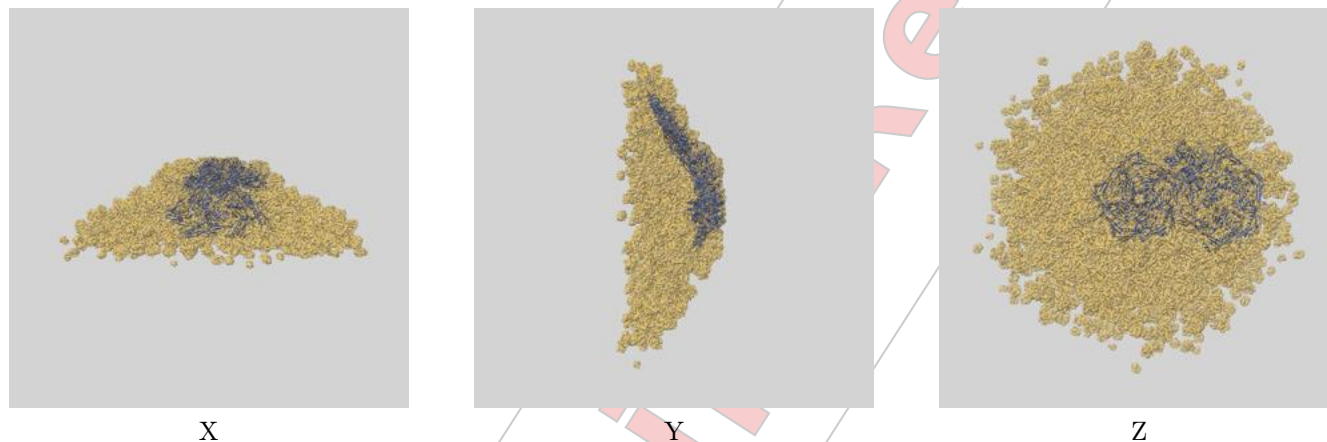
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.29	2.96
Unmasked-calculated*	3.49	4.02	3.55

*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 3.49 differs from the reported value 2.9 by more than 10 %

9 Map-model fit ⓘ

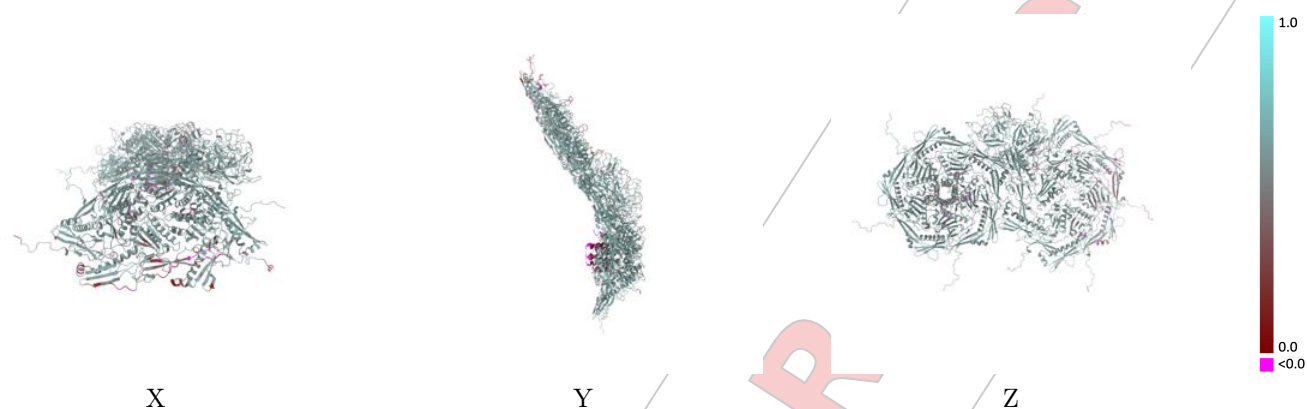
This section contains information regarding the fit between EMDB map EMD-44163 and PDB model 9B40. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ



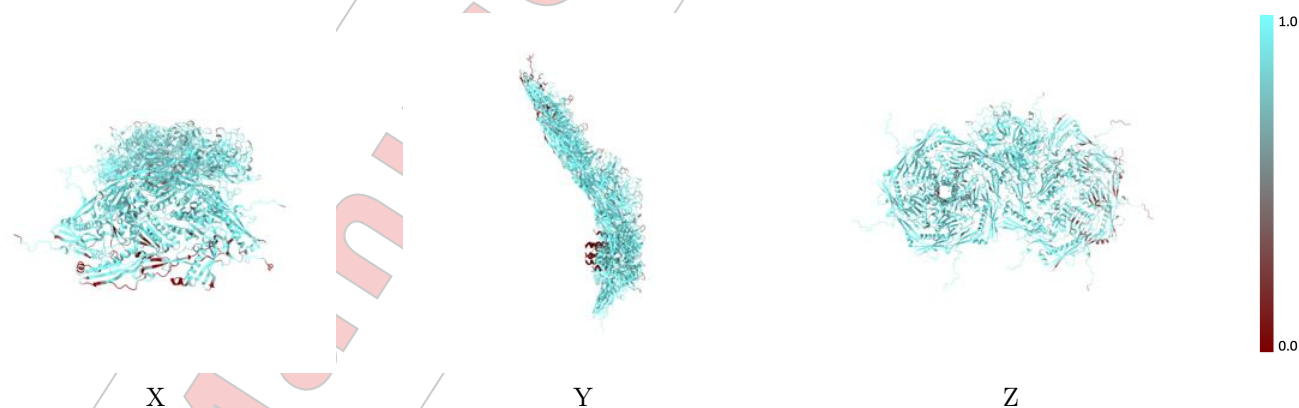
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



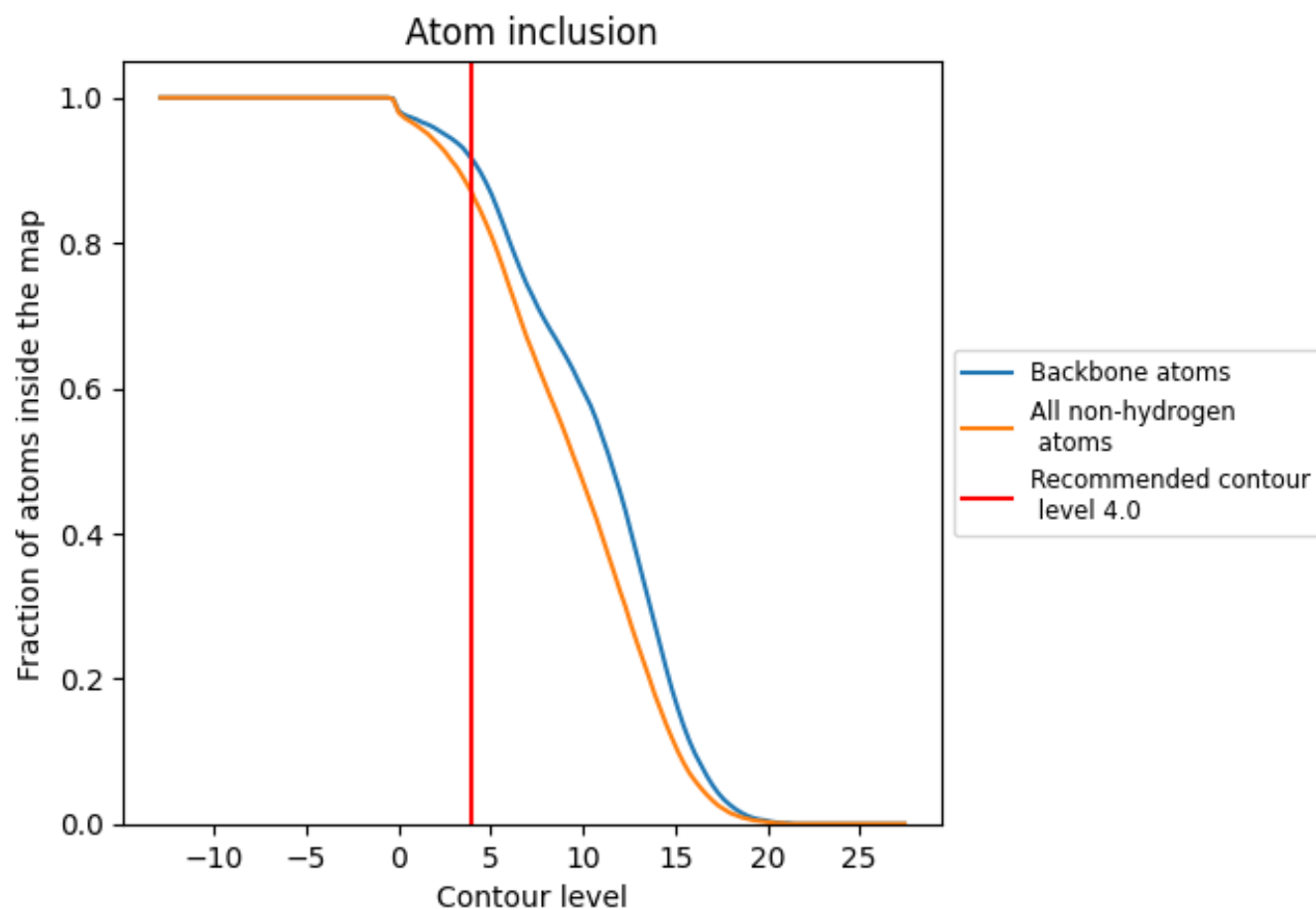
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.5510
A	 0.9220	 0.5730
B	 0.9250	 0.5780
C	 0.9230	 0.5730
D	 0.9250	 0.5770
E	 0.9250	 0.5770
F	 0.5720	 0.3820
G	 0.5610	 0.3860
H	 0.5830	 0.3970
I	 0.5720	 0.3910
J	 0.5400	 0.3690
K	 0.8750	 0.5530
L	 0.8960	 0.5720
M	 0.8890	 0.5630
N	 0.9320	 0.5830
O	 0.9260	 0.5750
P	 0.8770	 0.5570
Q	 0.8480	 0.5490
R	 0.7120	 0.4760
S	 0.7860	 0.5200

