

Full wwPDB EM Validation Report (i)

May 15, 2023 – 04:59 pm BST

PDB ID : 8B3Q

EMDB ID : EMD-15833

Title : CryoEM structure of the central filamentous region of the f1 filamentous bac-

teriophage, consisting of the major capsid protein pVIII

Authors: Conners, R.; McLaren, M.; Gold, V.A.M.

Deposited on : 2022-09-16

Resolution : 2.58 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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ : 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

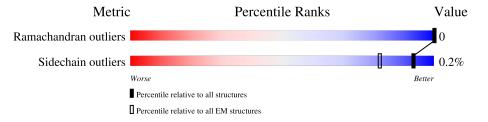
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 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 $(\# \mathrm{Entries})$	${ m EM~structures} \ (\#{ m Entries})$		
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 <=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	AAA	50	92%	8%
1	AaA	50	92%	8%
1	AbA	50	92%	8%
1	AcA	50	92%	8%
1	AdA	50	92%	8%
1	AeA	50	92%	8%
1	AfA	50	92%	8%
1	AgA	50	70% 30%	
1	AhA	50	92%	8%



Mol	Chain	Length	Quality of chain	
1	AiA	50	92%	8%
1	AjA	50	92%	8%
1	AkA	50	92%	8%
1	AlA	50	90%	8%
1	AmA	50	6%	
			92%	8%
1	AnA	50	92%	8%
1	BBB	50	92%	8%
1	BaB	50	92%	8%
1	BbB	50	92%	8%
1	BcB	50	92%	8%
1	BdB	50	92%	8%
1	BeB	50	92%	8%
1	BfB	50	92%	8%
1	BgB	50	70% 30%	
1	BhB	50	92%	8%
1	BiB	50	92%	8%
1	BjB	50	92%	8%
	BkB	50	<u>•</u>	
1			90%	
1	BlB	50	92% <mark>6%</mark>	8%
1	BmB	50	92%	8%
1	BnB	50	92%	8%
1	CCC	50	92%	8%
1	CaC	50	92%	8%
1	CbC	50	92%	8%
1	CcC	50	92%	8%



Mol	Chain	$oxed{ egin{array}{c} { m Previous} \\ { m Length} \end{array} }$	Quality of chain	
1	CdC	50	92%	8%
1	CeC	50	92%	8%
1	CfC	50	92%	8%
1	CgC	50	70% 30%	_
1	ChC	50	92%	8%
1	CiC	50	92%	8%
1	CjC	50	92%	8%
1	CkC	50	•	
			•	• 8%
1	ClC	50	92% 6%	8%
1	CmC	50	24%	8%
1	CnC	50	92%	8%
1	DDD	50	92%	8%
1	DaD	50	92%	8%
1	DbD	50	92%	8%
1	DcD	50	92%	8%
1	DdD	50	92%	8%
1	DeD	50	92%	8%
1	DfD	50	92%	8%
1	DgD	50	70% 30%	
1	DhD	50	92%	8%
1	DiD	50	92%	8%
1	DjD	50	92%	8%
1	DkD	50	90%	• 8%
1	DlD	50	92%	8%
1	DmD	50	<u>6%</u> 92%	8%



Mol	Chain	Length	Quality of chain	
	D D		24%	
1	DnD	50	92%	8%
1	EEE	50	92%	8%
1	EaE	50	92%	8%
1	EbE	50	92%	8%
1	EcE	50	92%	8%
1	EdE	50	92%	8%
1	EeE	50	92%	8%
1	EfE	50	92%	8%
1	EgE	50	70% 30	%
1	EhE	50	92%	8%
1	EiE	50	92%	8%
1	EjE	50	92%	8%
1	EkE	50	90%	. 8%
1	ElE	50	92%	8%
1	EmE	50	92%	8%
1	EnE	50	92%	8%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25095 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 Capsid protein G8P.

Mol	Chain	Residues		Ato	ms			AltConf	Trace
1	A A A	46	Total	С	N	О	S	0	0
1	AAA	40	340	223	53	62	2	0	0
1	DDD	46	Total	С	N	О	S	0	0
1	BBB	40	340	223	53	62	2	0	U
1	CCC	46	Total	С	N	О	S	0	0
1		40	340	223	53	62	2	0	0
1	DDD	46	Total	\mathbf{C}	N	Ο	S	0	0
1	סטט	40	340	223	53	62	2	0	U
1	EEE	46	Total	С	N	Ο	S	0	0
	DDD	10	340	223	53	62	2	· ·	U
1	AaA	46	Total	С	N	Ο	S	0	0
	71071	10	340	223	53	62	2	Ŭ	
1	BaB	46	Total	\mathbf{C}	N	Ο	S	0	0
	БаБ	10	340	223	53	62	2	Ů	Ů
1	CaC	46	Total	С	N	Ο	S	0	0
		10	340	223	53	62	2	Ŭ	Ů
1	DaD	46	Total	С	N	Ο	S	0	0
	Bab	10	340	223	53	62	2	Ü	
1	EaE	46	Total	С	N	Ο	S	0	0
	202	10	340	223	53	62	2	Ü	
1	AbA	46	Total	\mathbf{C}	N	Ο	S	0	0
	11011	10	340	223	53	62	2	Ü	Ů
1	BbB	46	Total	С	N	Ο	S	0	0
	ВоВ	10	340	223	53	62	2	Ü	Ů
1	CbC	46	Total	С	N	Ο	S	0	0
		10	340	223	53	62	2	Ü	
1	DbD	46	Total	С	N	Ο	S	0	0
		10	340	223	53	62	2	Ü	Ů
1	EbE	46	Total	С	N	Ο	S	0	0
		10	340	223	53	62	2		
1	AcA	46	Total	С	N	O	\mathbf{S}	0	0
	11011	10	340	223	53	62	2		
1	BcB	46	Total	С	N	Ο	\mathbf{S}	0	0
_			340	223	53	62	2		U



Mol	Chain	$oxed{ \mathbf{Residues} }$	9	Ato	ms			AltConf	Trace
1	0.0	4.0	Total	С	N	О	S	0	0
1	CcC	46	340	223	53	62	2	0	0
1	D D	4.6	Total	С	N	О	S	0	0
1	DcD	46	340	223	53	62	2	0	0
1	D. D	4.0	Total	С	N	О	S	0	0
1	EcE	46	340	223	53	62	2	0	0
1	٨٨٨	46	Total	С	N	О	S	0	0
1	AdA	40	340	223	53	62	2	U	U
1	BdB	46	Total	С	N	О	S	0	0
1	Dub	40	340	223	53	62	2		0
1	CdC	46	Total	С	N	О	S	0	0
1	CuC	40	340	223	53	62	2	U	0
1	DdD	46	Total	С	N	О	S	0	0
		40	340	223	53	62	2	U U	
1	EdE	46	Total	С	N	О	S	0	0
1	Eur	40	340	223	53	62	2	U	0
1	AeA	46	Total	С	N	Ο	S	0	0
1	AcA	40	340	223	53	62	2		U
1	BeB	46	Total	С	N	Ο	S	0	0
1	Den	40	340	223	53	62	2	0	U
1	CeC	46	Total	С	N	Ο	S	0	0
1	000	40	340	223	53	62	2	U	J 0
1	DeD	46	Total	С	N	Ο	S	0	0
1	DCD	40	340	223	53	62	2		
1	EeE	46	Total	С	N	Ο	S	0	0
1	LCL	10	340	223	53	62	2		0
1	AfA	46	Total	С	N	Ο	S	0	0
1	71171	10	340	223	53	62	2		0
1	BfB	46	Total	\mathbf{C}	N	Ο	S	0	0
1	DID	10	340	223	53	62	2		0
1	CfC	46	Total	С	N	Ο	S	0	0
	010	10	340	223	53	62	2		
1	DfD	46	Total	С	N	O	S	0	0
			340	223	53	62	2		Ŭ
1	EfE	46	Total	С	N	O	S	0	0
		-5	340	223	53	62	2		Ŭ,
1	AgA	35	Total	C	N	O	S	0	0
	J	_	259	172	40	45	2	0	-
1	BgB	35	Total	C	N	0	S	0	0
		_	259	172	40	45	2	-	
1	CgC	35	Total	C	N	0	S	0	0
	1 CgC		259	172	40	45	2	_	J



Mol	Chain	Residues	9	Ato	ms			AltConf	Trace
1			Total	С	N	О	S	0	
1	DgD	35	259	172	40	45	2	0	0
1	D-D	25	Total	С	N	О	S	0	0
1	EgE	35	259	172	40	45	2	0	0
1	Λ Ι. Λ	46	Total	С	N	О	S	0	0
1	AhA	40	340	223	53	62	2	0	0
1	BhB	46	Total	С	N	О	S	0	0
1	DIID	40	340	223	53	62	2	0	U
1	ChC	46	Total	С	N	О	S	0	0
1	CIIC	40	340	223	53	62	2	0	U
1	DhD	46	Total	С	N	О	S	0	0
1	עווע	40	340	223	53	62	2	0	U
1	EhE	46	Total	С	N	Ο	S	0	0
1	בוווט	40	340	223	53	62	2	0	
1	AiA	46	Total	С	N	О	S	0	0
1	AIA	40	340	223	53	62	2	0	U
1	BiB	46	Total	С	N	О	S	0	0
1	מומ	40	340	223	53	62	2	0	0
1	CiC	46	Total	С	N	О	S	0	0
1	CIC	40	340	223	53	62	2	0	U
1	DiD	46	Total	С	N	О	S	0	0
1	מוט	40	340	223	53	62	2	U	U
1	EiE	46	Total	С	N	Ο	S	0	0
1	12112	40	340	223	53	62	2	U	
1	AjA	46	Total	С	N	Ο	S	0	0
1	АјА	40	340	223	53	62	2	0	U
1	ВјВ	46	Total	\mathbf{C}	N	Ο	S	0	0
1	DJD	40	340	223	53	62	2	O	U
1	CjC	46	Total	\mathbf{C}	N	Ο	S	0	0
1	CjC	40	340	223	53	62	2	O	U
1	DjD	46	Total	\mathbf{C}	N	Ο	S	0	0
1	DjD	10	340	223	53	62	2	O	O
1	EjE	46	Total	С	N	Ο	S	0	0
1	D)D	10	340	223	53	62	2	O	O
1	AkA	46	Total	\mathbf{C}	N	Ο	\mathbf{S}	0	0
1	11111	10	340	223	53	62	2		
1	BkB	46	Total	С	N	Ο	S	0	0
1	2.1.0	10	340	223	53	62	2		0
1	CkC	46	Total	С	N	О	S	0	0
			340	223	53	62	2		
1	DkD	46	Total	С	N	O	S	0	0
			340	223	53	62	2		



Mol	Chain	Residues		Ato	ms			AltConf	Trace
1	DI D	4.0	Total	С	N	О	S	0	0
1	EkE	46	340	223	53	62	2	0	0
1	A 1 A	4.0	Total	С	N	О	S	0	0
1	AlA	46	340	223	53	62	2	0	0
1	DID	46	Total	С	N	О	S	0	0
1	BlB	40	340	223	53	62	2	0	U
1	ClC	46	Total	С	N	О	S	0	0
1	CIC	40	340	223	53	62	2	0	U
1	DlD	46	Total	С	N	О	S	0	0
1	עוע	40	340	223	53	62	2	0	U
1	ElE	46	Total	С	N	Ο	S	0	0
1		40	340	223	53	62	2	0	0
1	AmA	46	Total	С	N	Ο	S	0	0
1	7 11117 1	40	340	223	53	62	2	U	U
1	BmB	46	Total	С	N	Ο	S	0	0
1	Dillib	40	340	223	53	62	2	Ü	
1	CmC	46	Total	С	N	О	S	0	0
1	Onic	10	340	223	53	62	2	Ů	
1	DmD	46	Total	С	N	О	S	0	0
1	Dilib	10	340	223	53	62	2	Ŭ	0
1	EmE	46	Total	С	N	Ο	S	0	0
	Billib	10	340	223	53	62	2	Ů	
1	AnA	46	Total	С	N	О	S	0	0
	111111	10	340	223	53	62	2	Ŭ	
1	BnB	46	Total	С	N	О	S	0	0
		10	340	223	53	62	2	Ů	
1	CnC	46	Total	С	N	0	S	0	0
			340	223	53	62	2		
1	DnD	46	Total	С	N	0	S	0	0
			340	223	53	62	2		
1	EnE	46	Total	С	N	0	S	0	0
		10	340	223	53	62	2	U	

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	21	MET	TYR	engineered mutation	UNP P69540
BBB	21	MET	TYR	engineered mutation	UNP P69540
CCC	21	MET	TYR	engineered mutation	UNP P69540
DDD	21	MET	TYR	engineered mutation	UNP P69540
EEE	21	MET	TYR	engineered mutation	UNP P69540
AaA	21	MET	TYR	engineered mutation	UNP P69540
BaB	21	MET	TYR	engineered mutation	UNP P69540



Chain	Residue	Modelled	Actual	Comment	Reference
CaC	21	MET	TYR	engineered mutation	UNP P69540
DaD	21	MET	TYR	engineered mutation	UNP P69540
EaE	21	MET	TYR	engineered mutation	UNP P69540
AbA	21	MET	TYR	engineered mutation	UNP P69540
BbB	21	MET	TYR	engineered mutation	UNP P69540
CbC	21	MET	TYR	engineered mutation	UNP P69540
DbD	21	MET	TYR	engineered mutation	UNP P69540
EbE	21	MET	TYR	engineered mutation	UNP P69540
AcA	21	MET	TYR	engineered mutation	UNP P69540
BcB	21	MET	TYR	engineered mutation	UNP P69540
CcC	21	MET	TYR	engineered mutation	UNP P69540
DcD	21	MET	TYR	engineered mutation	UNP P69540
EcE	21	MET	TYR	engineered mutation	UNP P69540
AdA	21	MET	TYR	engineered mutation	UNP P69540
BdB	21	MET	TYR	engineered mutation	UNP P69540
CdC	21	MET	TYR	engineered mutation	UNP P69540
DdD	21	MET	TYR	engineered mutation	UNP P69540
EdE	21	MET	TYR	engineered mutation	UNP P69540
AeA	21	MET	TYR	engineered mutation	UNP P69540
BeB	21	MET	TYR	engineered mutation	UNP P69540
CeC	21	MET	TYR	engineered mutation	UNP P69540
DeD	21	MET	TYR	engineered mutation	UNP P69540
EeE	21	MET	TYR	engineered mutation	UNP P69540
AfA	21	MET	TYR	engineered mutation	UNP P69540
BfB	21	MET	TYR	engineered mutation	UNP P69540
CfC	21	MET	TYR	engineered mutation	UNP P69540
DfD	21	MET	TYR	engineered mutation	UNP P69540
EfE	21	MET	TYR	engineered mutation	UNP P69540
AgA	21	MET	TYR	engineered mutation	UNP P69540
BgB	21	MET	TYR	engineered mutation	UNP P69540
CgC	21	MET	TYR	engineered mutation	UNP P69540
DgD	21	MET	TYR	engineered mutation	UNP P69540
EgE	21	MET	TYR	engineered mutation	UNP P69540
AhA	21	MET	TYR	engineered mutation	UNP P69540
BhB	21	MET	TYR	engineered mutation	UNP P69540
ChC	21	MET	TYR	engineered mutation	UNP P69540
DhD	21	MET	TYR	engineered mutation	UNP P69540
EhE	21	MET	TYR	engineered mutation	UNP P69540
AiA	21	MET	TYR	engineered mutation	UNP P69540
BiB	21	MET	TYR	engineered mutation	UNP P69540
CiC	21	MET	TYR	engineered mutation	UNP P69540
DiD	21	MET	TYR	engineered mutation	UNP P69540

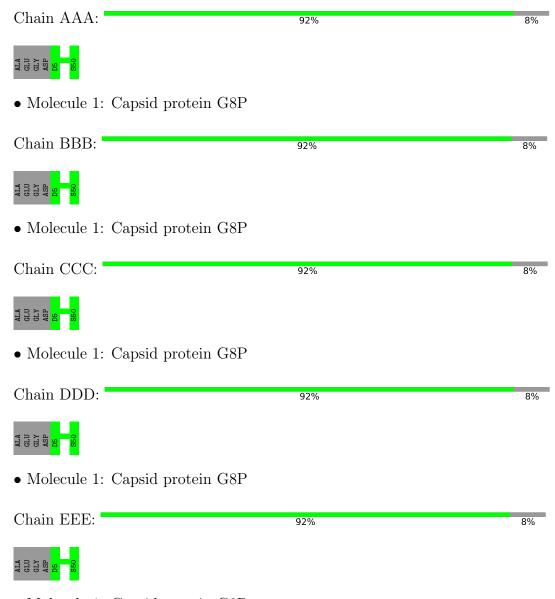


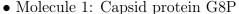
Chain	Residue	Modelled	Actual	Comment	Reference
EiE	21	MET	TYR	engineered mutation	UNP P69540
AjA	21	MET	TYR	engineered mutation	UNP P69540
BjB	21	MET	TYR	engineered mutation	UNP P69540
CjC	21	MET	TYR	engineered mutation	UNP P69540
DjD	21	MET	TYR	engineered mutation	UNP P69540
EjE	21	MET	TYR	engineered mutation	UNP P69540
AkA	21	MET	TYR	engineered mutation	UNP P69540
BkB	21	MET	TYR	engineered mutation	UNP P69540
CkC	21	MET	TYR	engineered mutation	UNP P69540
DkD	21	MET	TYR	engineered mutation	UNP P69540
EkE	21	MET	TYR	engineered mutation	UNP P69540
AlA	21	MET	TYR	engineered mutation	UNP P69540
BlB	21	MET	TYR	engineered mutation	UNP P69540
ClC	21	MET	TYR	engineered mutation	UNP P69540
DlD	21	MET	TYR	engineered mutation	UNP P69540
ElE	21	MET	TYR	engineered mutation	UNP P69540
AmA	21	MET	TYR	engineered mutation	UNP P69540
BmB	21	MET	TYR	engineered mutation	UNP P69540
CmC	21	MET	TYR	engineered mutation	UNP P69540
DmD	21	MET	TYR	engineered mutation	UNP P69540
EmE	21	MET	TYR	engineered mutation	UNP P69540
AnA	21	MET	TYR	engineered mutation	UNP P69540
BnB	21	MET	TYR	engineered mutation	UNP P69540
CnC	21	MET	TYR	engineered mutation	UNP P69540
DnD	21	MET	TYR	engineered mutation	UNP P69540
EnE	21	MET	TYR	engineered mutation	UNP P69540



3 Residue-property plots (i)

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





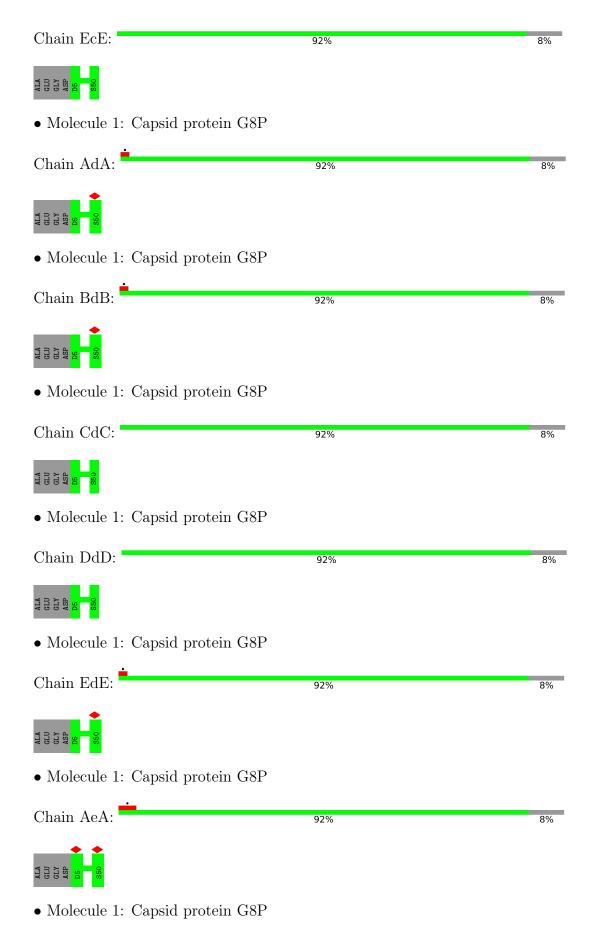


Chain AaA:	92%	8%
ALA GLU GLU GLU ASP		
• Molecule 1: Capsid protein G8P		
Chain BaB:	92%	8%
ALA GLU GLU GLV ASP DS SSO		
• Molecule 1: Capsid protein G8P		
Chain CaC:	92%	8%
ALA GLU GLU GLY ASP ASP SS0		
• Molecule 1: Capsid protein G8P		
Chain DaD:	92%	8%
ALA GIU GIU GIV ASP BS SSO		
• Molecule 1: Capsid protein G8P		
Chain EaE:	92%	8%
ALA ASP DS SSO		
• Molecule 1: Capsid protein G8P		
Chain AbA:	92%	8%
ALA GLU GLU GLU ASP		
• Molecule 1: Capsid protein G8P		
Chain BbB:	92%	8%
ALA GLU GLU GLU ASP		
Molecule 1: Capsid protein G8P		

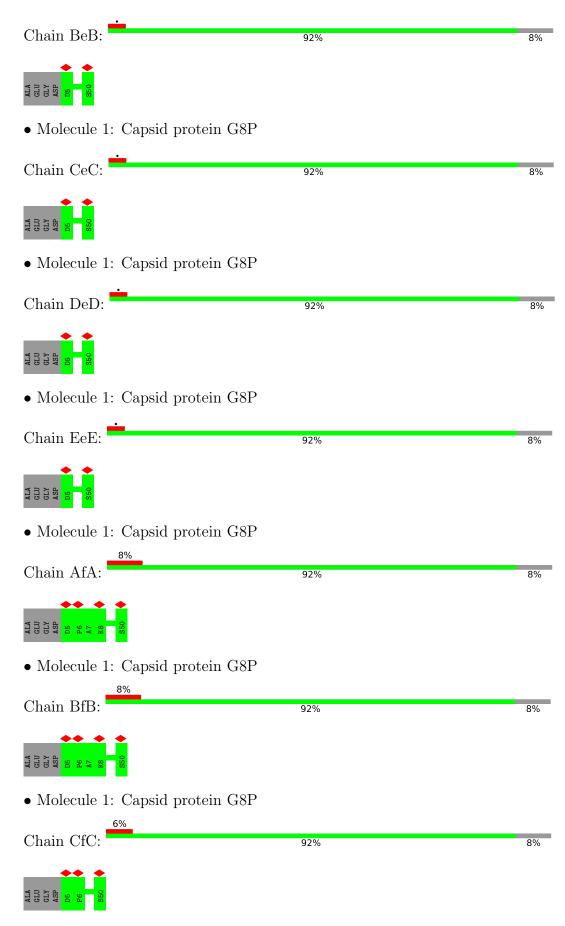


Chain CbC:	92%	8%
ALA GLU GLU GLU GLU ASP		
• Molecule 1: Capsid protein G8P		
Chain DbD:	92%	8%
ALA GLU GLY ASP DS		
• Molecule 1: Capsid protein G8P		
Chain EbE:	92%	8%
ALA GLU GLY ASP DS SSO		
• Molecule 1: Capsid protein G8P		
Chain AcA:	92%	8%
ALA GLU GLY ASP DS SE0		
• Molecule 1: Capsid protein G8P		
Chain BcB:	92%	8%
ALA GLU GLU GLY ASP		
• Molecule 1: Capsid protein G8P		
Chain CcC:	92%	8%
ALA GLU GLU GLY ASP SSO		
• Molecule 1: Capsid protein G8P		
Chain DcD:	92%	8%
ALA GLU GLU GLY ASP DS SSO		
• Molecule 1: Capsid protein G8P		

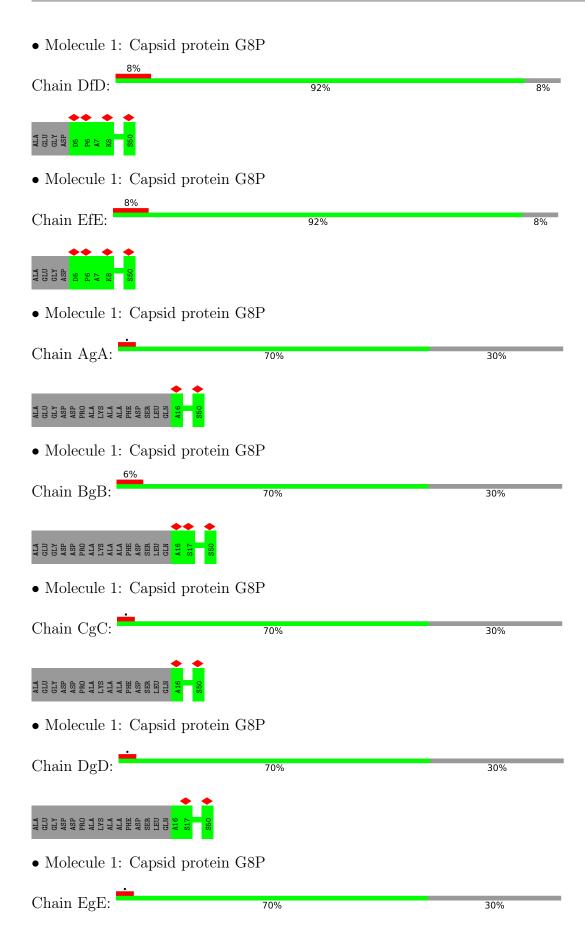








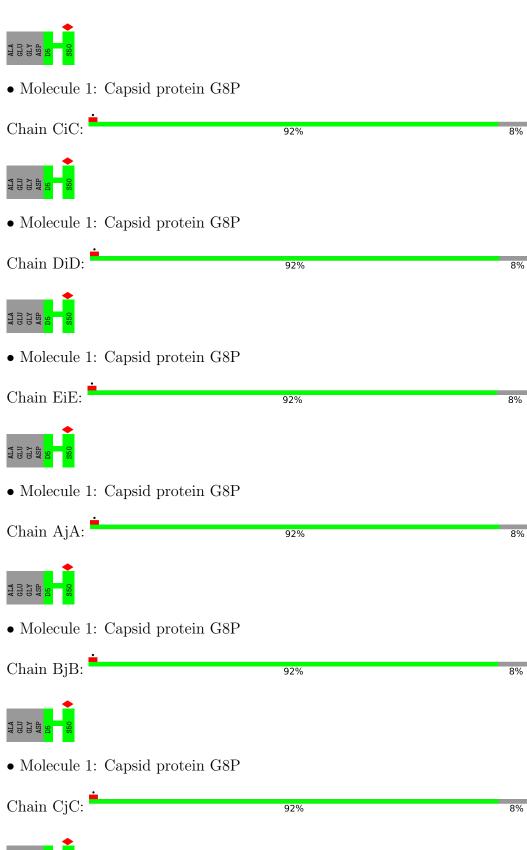






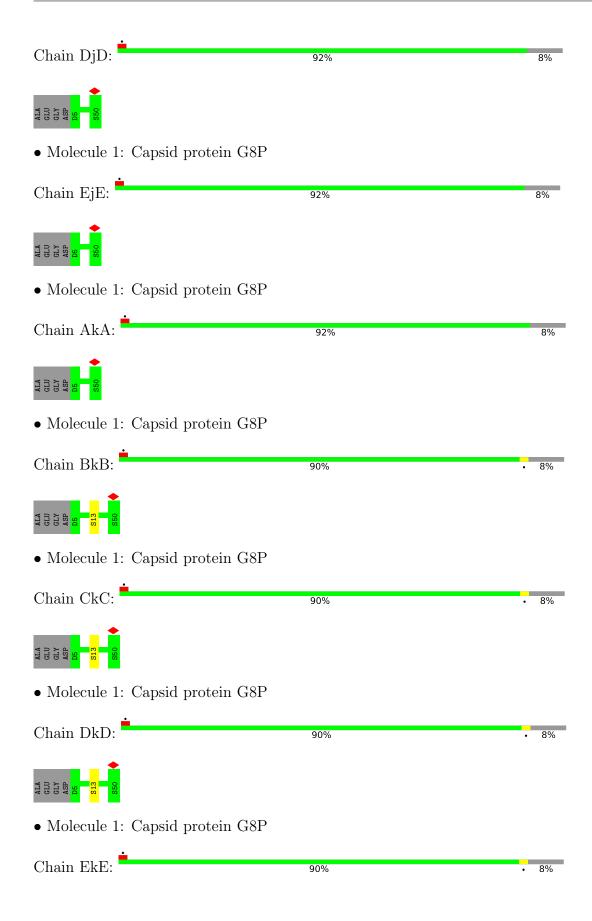




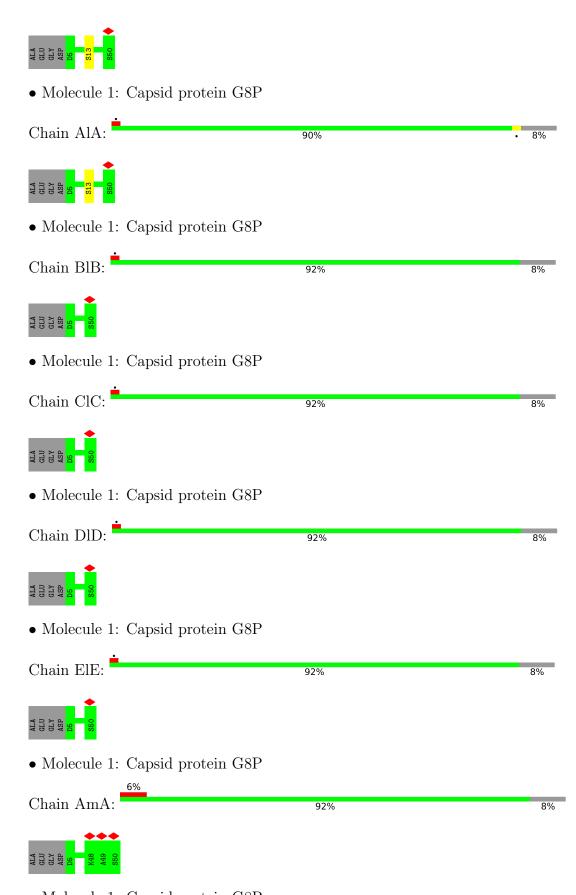




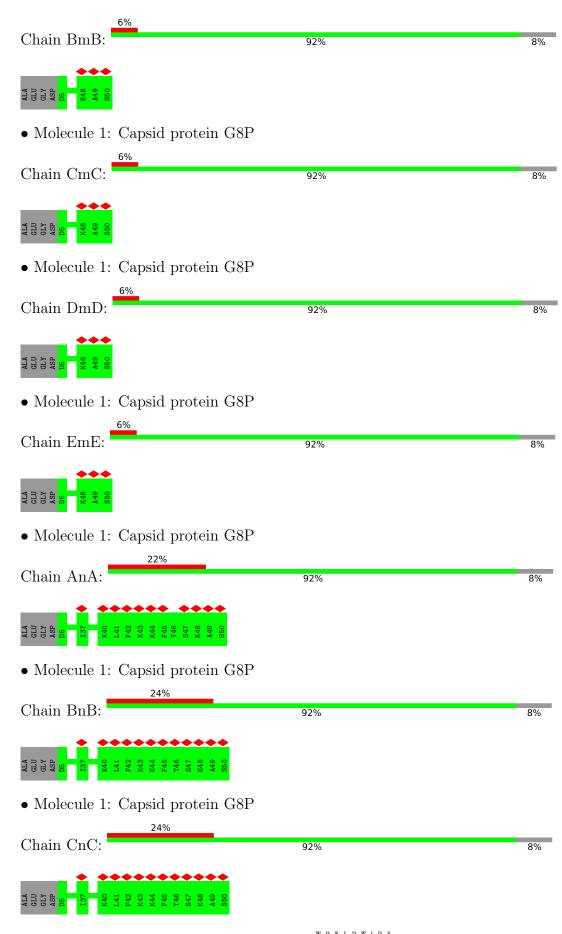




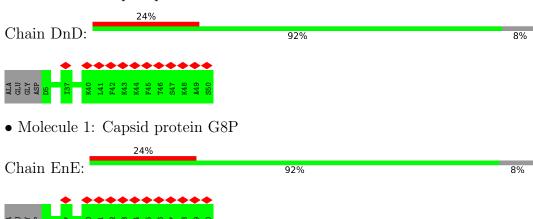














4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=37.437°, rise=16.599 Å,	Depositor
	axial sym=C5	
Number of segments used	1139813	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.696	Depositor
Minimum map value	-0.218	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	330.36, 330.36, 330.36	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1012, 1.1012, 1.1012	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).

Mal	Chain	Bond	lengths	Bond	angles
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AAA	0.56	0/346	0.76	0/465
1	AaA	0.56	0/346	0.75	0/465
1	AbA	0.54	0/346	0.75	0/465
1	AcA	0.52	0/346	0.74	0/465
1	AdA	0.50	0/346	0.72	0/465
1	AeA	0.47	0/346	0.70	0/465
1	AfA	0.44	0/346	0.68	0/465
1	AgA	0.50	0/263	0.71	0/352
1	AhA	0.56	0/346	0.75	0/465
1	AiA	0.54	0/346	0.76	0/465
1	AjA	0.53	0/346	0.75	0/465
1	AkA	0.50	0/346	0.72	0/465
1	AlA	0.47	0/346	0.69	0/465
1	AmA	0.44	0/346	0.65	0/465
1	AnA	0.40	0/346	0.63	0/465
1	BBB	0.56	0/346	0.75	0/465
1	BaB	0.56	0/346	0.77	0/465
1	BbB	0.54	0/346	0.75	0/465
1	BcB	0.53	0/346	0.74	0/465
1	BdB	0.50	0/346	0.73	0/465
1	BeB	0.47	0/346	0.70	0/465
1	BfB	0.44	0/346	0.68	0/465
1	BgB	0.48	0/263	0.70	0/352
1	BhB	0.56	0/346	0.76	0/465
1	BiB	0.55	0/346	0.76	0/465
1	BjB	0.53	0/346	0.74	0/465
1	BkB	0.50	0/346	0.72	0/465
1	BlB	0.47	0/346	0.69	0/465
1	BmB	0.44	0/346	0.66	0/465
1	BnB	0.41	0/346	0.63	0/465
1	CCC	0.57	0/346	0.76	0/465
1	CaC	0.55	0/346	0.76	0/465
1	CbC	0.55	0/346	0.75	0/465
1	CcC	0.53	0/346	0.74	0/465



		Rond	lengths	Rond	angles
Mol	Chain	RMSZ	# Z >5	RMSZ	angles $ \# Z > 5$
1	C4C				
1	CdC	0.50	0/346	0.72	0/465
1	CeC	0.47	0/346	0.70	0/465
	CfC	0.44	0/346	0.68	0/465
1	CgC	0.47	0/263	0.71	0/352
1	ChC	0.56	0/346	0.76	0/465
1	CiC	0.55	0/346	0.76	0/465
1	CjC	0.53	0/346	0.74	0/465
1	CkC	0.50	0/346	0.72	0/465
1	ClC	0.48	0/346	0.70	0/465
1	CmC	0.44	0/346	0.66	0/465
1	CnC	0.41	0/346	0.64	0/465
1	DDD	0.57	0/346	0.77	0/465
1	DaD	0.56	0/346	0.76	0/465
1	DbD	0.55	0/346	0.76	0/465
1	DcD	0.53	0/346	0.73	0/465
1	DdD	0.50	0/346	0.73	0/465
1	DeD	0.47	0/346	0.70	0/465
1	DfD	0.44	0/346	0.68	0/465
1	DgD	0.49	0/263	0.71	0/352
1	DhD	0.56	0/346	0.76	0/465
1	DiD	0.54	0/346	0.76	0/465
1	DjD	0.53	0/346	0.75	0/465
1	DkD	0.50	0/346	0.72	0/465
1	DlD	0.48	0/346	0.68	0/465
1	DmD	0.44	0/346	0.66	0/465
1	DnD	0.41	0/346	0.64	0/465
1	EEE	0.56	0/346	0.76	0/465
1	EaE	0.56	0/346	0.77	0/465
1	EbE	0.55	0/346	0.75	0/465
1	EcE	0.52	0/346	0.74	0/465
1	EdE	0.50	0/346	0.72	0/465
1	EeE	0.47	0/346	0.70	0/465
1	EfE	0.44	0/346	0.68	0/465
1	EgE	0.50	0/263	0.72	0/352
1	EhE	0.56	0/346	0.76	0/465
1	EiE	0.54	0/346	0.76	0/465
1	EjE	0.53	0/346	0.74	0/465
1	EkE	0.50	0/346	0.70	0/465
1	ElE	0.47	0/346	0.69	0/465
1	EmE	0.44	0/346	0.65	0/465
1	EnE	0.41	0/346	0.64	0/465
All	All	0.51	0/25535	0.72	0/34310
			,	. –	,



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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	AAA	44/50~(88%)	44 (100%)	0	0	100	100
1	AaA	44/50 (88%)	44 (100%)	0	0	100	100
1	AbA	44/50 (88%)	44 (100%)	0	0	100	100
1	AcA	44/50 (88%)	44 (100%)	0	0	100	100
1	AdA	44/50 (88%)	44 (100%)	0	0	100	100
1	AeA	44/50 (88%)	44 (100%)	0	0	100	100
1	AfA	44/50 (88%)	44 (100%)	0	0	100	100
1	AgA	33/50 (66%)	33 (100%)	0	0	100	100
1	AhA	44/50 (88%)	44 (100%)	0	0	100	100
1	AiA	44/50 (88%)	44 (100%)	0	0	100	100
1	AjA	44/50 (88%)	44 (100%)	0	0	100	100
1	AkA	44/50 (88%)	44 (100%)	0	0	100	100
1	AlA	44/50 (88%)	44 (100%)	0	0	100	100
1	AmA	44/50 (88%)	44 (100%)	0	0	100	100
1	AnA	44/50 (88%)	44 (100%)	0	0	100	100
1	BBB	44/50 (88%)	44 (100%)	0	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	BaB	44/50~(88%)	44 (100%)	0	0	100	100
1	BbB	44/50~(88%)	44 (100%)	0	0	100	100
1	BcB	44/50~(88%)	44 (100%)	0	0	100	100
1	BdB	44/50~(88%)	44 (100%)	0	0	100	100
1	BeB	44/50 (88%)	44 (100%)	0	0	100	100
1	BfB	44/50 (88%)	44 (100%)	0	0	100	100
1	BgB	33/50 (66%)	33 (100%)	0	0	100	100
1	BhB	44/50 (88%)	44 (100%)	0	0	100	100
1	BiB	44/50 (88%)	44 (100%)	0	0	100	100
1	BjB	44/50~(88%)	44 (100%)	0	0	100	100
1	BkB	44/50~(88%)	44 (100%)	0	0	100	100
1	BlB	44/50~(88%)	44 (100%)	0	0	100	100
1	BmB	44/50~(88%)	44 (100%)	0	0	100	100
1	BnB	44/50~(88%)	44 (100%)	0	0	100	100
1	CCC	44/50~(88%)	44 (100%)	0	0	100	100
1	CaC	44/50~(88%)	44 (100%)	0	0	100	100
1	CbC	44/50~(88%)	44 (100%)	0	0	100	100
1	CcC	44/50~(88%)	44 (100%)	0	0	100	100
1	CdC	44/50~(88%)	44 (100%)	0	0	100	100
1	CeC	44/50~(88%)	44 (100%)	0	0	100	100
1	CfC	44/50 (88%)	44 (100%)	0	0	100	100
1	CgC	33/50~(66%)	33 (100%)	0	0	100	100
1	ChC	44/50 (88%)	44 (100%)	0	0	100	100
1	CiC	44/50~(88%)	44 (100%)	0	0	100	100
1	CjC	44/50 (88%)	44 (100%)	0	0	100	100
1	CkC	44/50 (88%)	44 (100%)	0	0	100	100
1	ClC	44/50 (88%)	44 (100%)	0	0	100	100
1	CmC	44/50 (88%)	44 (100%)	0	0	100	100
1	CnC	44/50 (88%)	44 (100%)	0	0	100	100
1	DDD	44/50 (88%)	44 (100%)	0	0	100	100
1	DaD	44/50 (88%)	44 (100%)	0	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	DbD	44/50 (88%)	44 (100%)	0	0	100	100
1	DcD	44/50 (88%)	44 (100%)	0	0	100	100
1	DdD	44/50 (88%)	44 (100%)	0	0	100	100
1	DeD	44/50 (88%)	44 (100%)	0	0	100	100
1	DfD	44/50 (88%)	44 (100%)	0	0	100	100
1	DgD	33/50 (66%)	33 (100%)	0	0	100	100
1	DhD	44/50 (88%)	44 (100%)	0	0	100	100
1	DiD	44/50 (88%)	44 (100%)	0	0	100	100
1	DjD	44/50 (88%)	44 (100%)	0	0	100	100
1	DkD	44/50 (88%)	44 (100%)	0	0	100	100
1	DlD	44/50 (88%)	44 (100%)	0	0	100	100
1	DmD	44/50 (88%)	44 (100%)	0	0	100	100
1	DnD	44/50 (88%)	44 (100%)	0	0	100	100
1	EEE	44/50 (88%)	44 (100%)	0	0	100	100
1	EaE	44/50 (88%)	44 (100%)	0	0	100	100
1	EbE	44/50 (88%)	44 (100%)	0	0	100	100
1	EcE	44/50 (88%)	44 (100%)	0	0	100	100
1	EdE	44/50 (88%)	44 (100%)	0	0	100	100
1	EeE	44/50 (88%)	44 (100%)	0	0	100	100
1	EfE	44/50 (88%)	44 (100%)	0	0	100	100
1	EgE	33/50 (66%)	33 (100%)	0	0	100	100
1	EhE	44/50 (88%)	44 (100%)	0	0	100	100
1	EiE	44/50 (88%)	44 (100%)	0	0	100	100
1	EjE	44/50 (88%)	44 (100%)	0	0	100	100
1	EkE	44/50 (88%)	44 (100%)	0	0	100	100
1	ElE	44/50 (88%)	44 (100%)	0	0	100	100
1	EmE	44/50 (88%)	44 (100%)	0	0	100	100
1	EnE	44/50 (88%)	44 (100%)	0	0	100	100
All	All	3245/3750 (86%)	3245 (100%)	0	0	100	100

There are no Ramachandran outliers to report. $\,$



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	$\overline{\text{ntiles}}$
1	AAA	34/36~(94%)	34 (100%)	0	100	100
1	AaA	34/36~(94%)	34 (100%)	0	100	100
1	AbA	34/36 (94%)	34 (100%)	0	100	100
1	AcA	34/36 (94%)	34 (100%)	0	100	100
1	AdA	34/36 (94%)	34 (100%)	0	100	100
1	AeA	34/36 (94%)	34 (100%)	0	100	100
1	AfA	34/36 (94%)	34 (100%)	0	100	100
1	AgA	26/36 (72%)	26 (100%)	0	100	100
1	AhA	34/36 (94%)	34 (100%)	0	100	100
1	AiA	34/36 (94%)	34 (100%)	0	100	100
1	AjA	34/36 (94%)	34 (100%)	0	100	100
1	AkA	34/36 (94%)	34 (100%)	0	100	100
1	AlA	34/36 (94%)	33 (97%)	1 (3%)	42	66
1	AmA	34/36 (94%)	34 (100%)	0	100	100
1	AnA	34/36 (94%)	34 (100%)	0	100	100
1	BBB	34/36 (94%)	34 (100%)	0	100	100
1	BaB	34/36 (94%)	34 (100%)	0	100	100
1	BbB	34/36 (94%)	34 (100%)	0	100	100
1	BcB	34/36 (94%)	34 (100%)	0	100	100
1	BdB	34/36 (94%)	34 (100%)	0	100	100
1	BeB	34/36 (94%)	34 (100%)	0	100	100
1	BfB	34/36 (94%)	34 (100%)	0	100	100
1	BgB	$26/36 \ (72\%)$	26 (100%)	0	100	100
1	BhB	34/36 (94%)	34 (100%)	0	100	100
1	BiB	34/36 (94%)	34 (100%)	0	100	100
1	BjB	34/36 (94%)	34 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	BkB	34/36~(94%)	33 (97%)	1 (3%)	42	66
1	BlB	34/36~(94%)	34 (100%)	0	100	100
1	BmB	34/36~(94%)	34 (100%)	0	100	100
1	BnB	34/36~(94%)	34 (100%)	0	100	100
1	CCC	34/36~(94%)	34 (100%)	0	100	100
1	CaC	34/36 (94%)	34 (100%)	0	100	100
1	CbC	34/36~(94%)	34 (100%)	0	100	100
1	CcC	34/36 (94%)	34 (100%)	0	100	100
1	CdC	34/36~(94%)	34 (100%)	0	100	100
1	CeC	34/36 (94%)	34 (100%)	0	100	100
1	CfC	34/36 (94%)	34 (100%)	0	100	100
1	CgC	26/36 (72%)	26 (100%)	0	100	100
1	ChC	34/36 (94%)	34 (100%)	0	100	100
1	CiC	34/36 (94%)	34 (100%)	0	100	100
1	CjC	34/36 (94%)	34 (100%)	0	100	100
1	CkC	34/36 (94%)	33 (97%)	1 (3%)	42	66
1	ClC	34/36 (94%)	34 (100%)	0	100	100
1	CmC	34/36 (94%)	34 (100%)	0	100	100
1	CnC	34/36 (94%)	34 (100%)	0	100	100
1	DDD	34/36 (94%)	34 (100%)	0	100	100
1	DaD	34/36 (94%)	34 (100%)	0	100	100
1	DbD	34/36 (94%)	34 (100%)	0	100	100
1	DcD	34/36 (94%)	34 (100%)	0	100	100
1	DdD	34/36 (94%)	34 (100%)	0	100	100
1	DeD	34/36 (94%)	34 (100%)	0	100	100
1	DfD	34/36 (94%)	34 (100%)	0	100	100
1	DgD	26/36 (72%)	26 (100%)	0	100	100
1	DhD	34/36 (94%)	34 (100%)	0	100	100
1	DiD	34/36 (94%)	34 (100%)	0	100	100
1	DjD	34/36 (94%)	34 (100%)	0	100	100
1	DkD	34/36 (94%)	33 (97%)	1 (3%)	42	66



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	DlD	34/36~(94%)	34 (100%)	0	100	100
1	DmD	34/36~(94%)	34 (100%)	0	100	100
1	DnD	34/36~(94%)	34 (100%)	0	100	100
1	EEE	34/36 (94%)	34 (100%)	0	100	100
1	EaE	34/36 (94%)	34 (100%)	0	100	100
1	EbE	34/36 (94%)	34 (100%)	0	100	100
1	EcE	34/36 (94%)	34 (100%)	0	100	100
1	EdE	34/36 (94%)	34 (100%)	0	100	100
1	EeE	34/36 (94%)	34 (100%)	0	100	100
1	EfE	34/36 (94%)	34 (100%)	0	100	100
1	EgE	26/36 (72%)	26 (100%)	0	100	100
1	EhE	34/36 (94%)	34 (100%)	0	100	100
1	EiE	34/36 (94%)	34 (100%)	0	100	100
1	EjE	34/36 (94%)	34 (100%)	0	100	100
1	EkE	34/36 (94%)	33 (97%)	1 (3%)	42	66
1	ElE	34/36 (94%)	34 (100%)	0	100	100
1	EmE	34/36 (94%)	34 (100%)	0	100	100
1	EnE	34/36 (94%)	34 (100%)	0	100	100
All	All	2510/2700 (93%)	2505 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BkB	13	SER
1	CkC	13	SER
1	DkD	13	SER
1	EkE	13	SER
1	AlA	13	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.



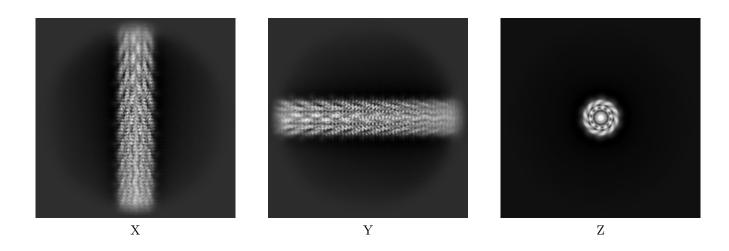
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15833. These allow visual inspection of the internal detail of the map and identification of artifacts.

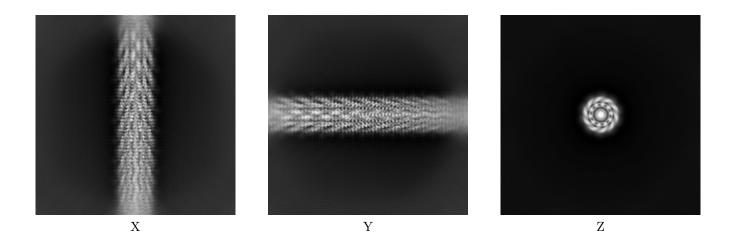
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

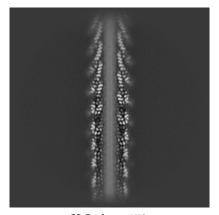


The images above show the map projected in three orthogonal directions.

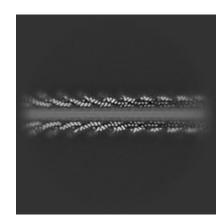


6.2 Central slices (i)

6.2.1 Primary map





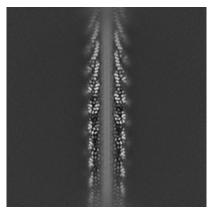


Y Index: 150

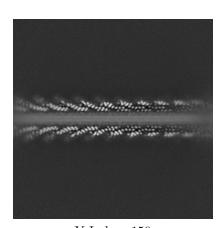


Z Index: 150

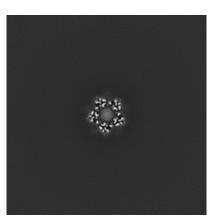
6.2.2 Raw map



X Index: 150



Y Index: 150



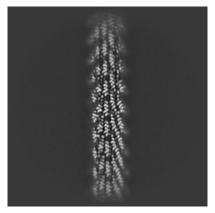
Z Index: 150

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

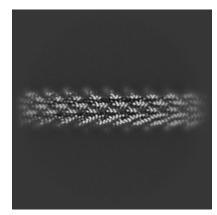


6.3 Largest variance slices (i)

6.3.1 Primary map





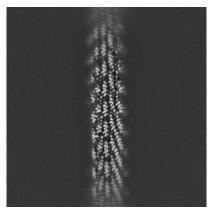


Y Index: 137

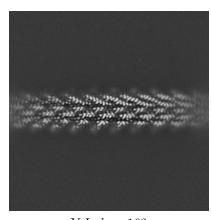


Z Index: 147

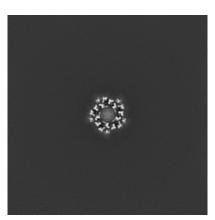
6.3.2 Raw map



X Index: 135



Y Index: 163



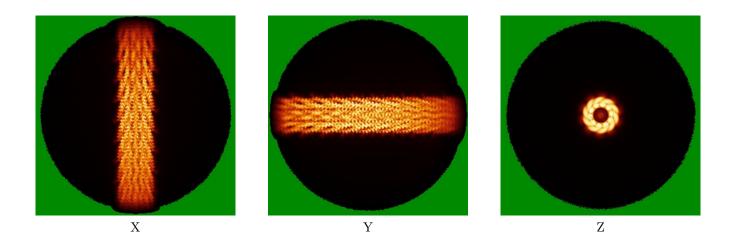
Z Index: 147

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

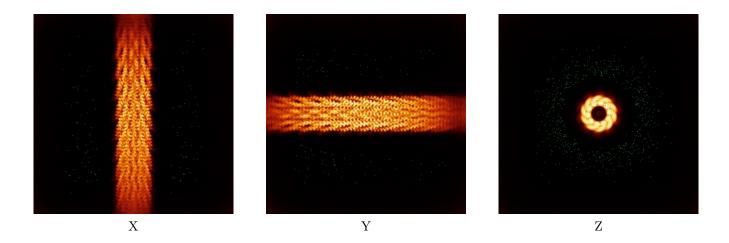


6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map

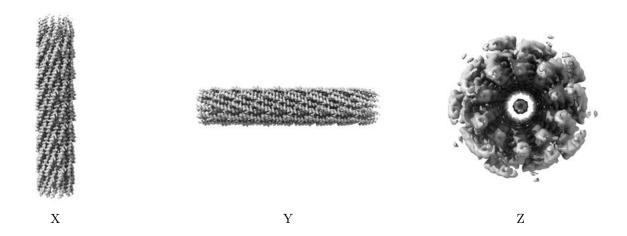


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



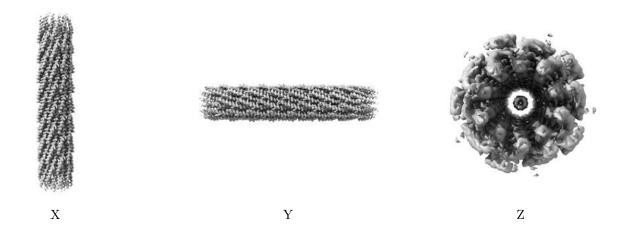
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

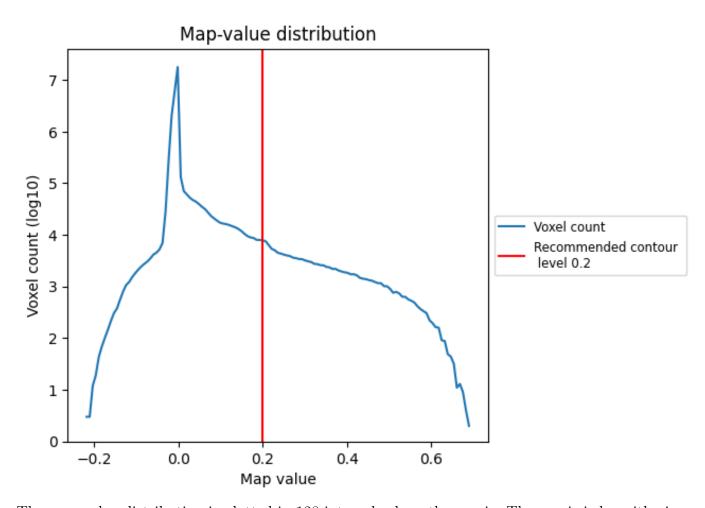
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

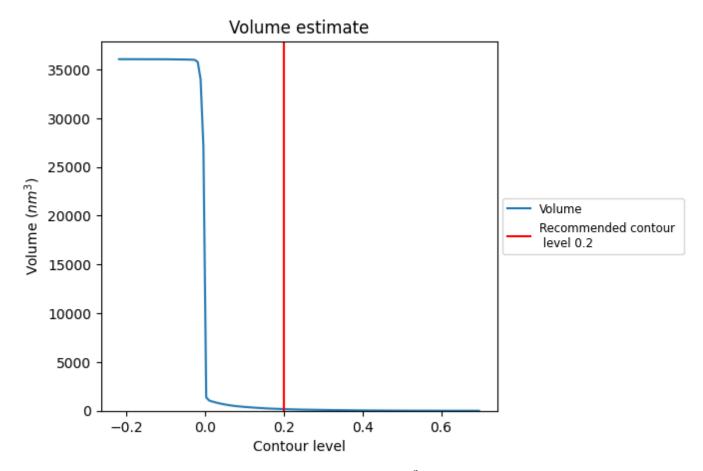
7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)

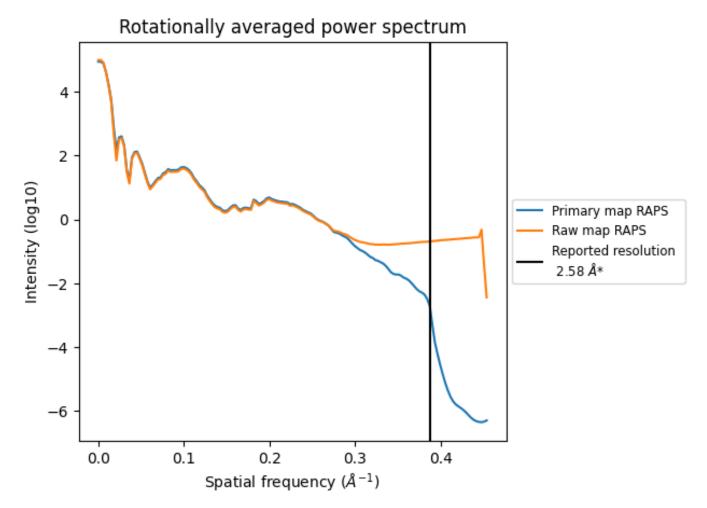


The volume at the recommended contour level is $173~\mathrm{nm}^3$; this corresponds to an approximate mass of $156~\mathrm{kDa}$.

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



7.3 Rotationally averaged power spectrum (i)



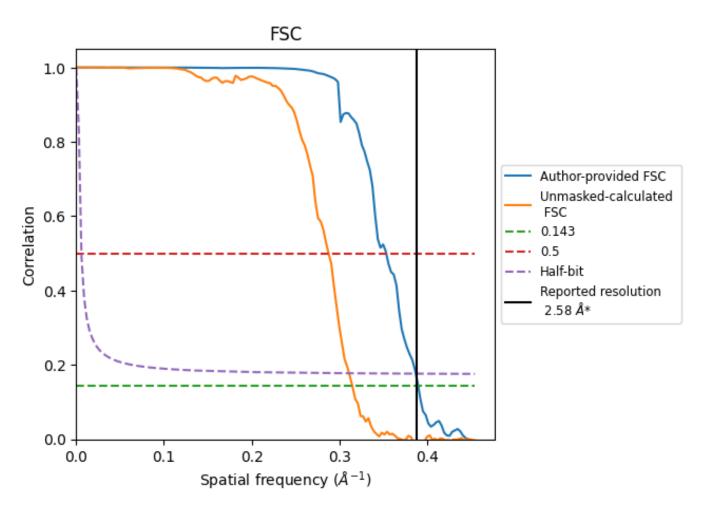
^{*}Reported resolution corresponds to spatial frequency of 0.388 $\rm \mathring{A}^{-1}$



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 0.388 $\rm \mathring{A}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
rtesolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.83	2.59
Unmasked-calculated*	3.18	3.48	3.22

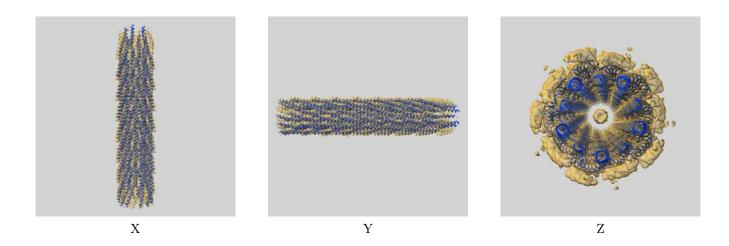
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.58 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15833 and PDB model 8B3Q. Per-residue inclusion information can be found in section 3 on page 12.

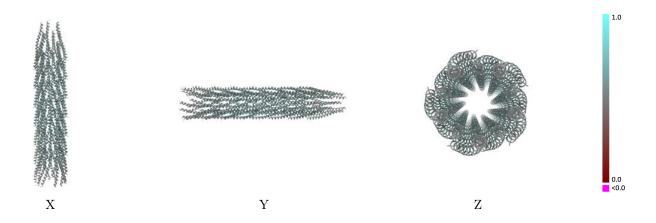
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

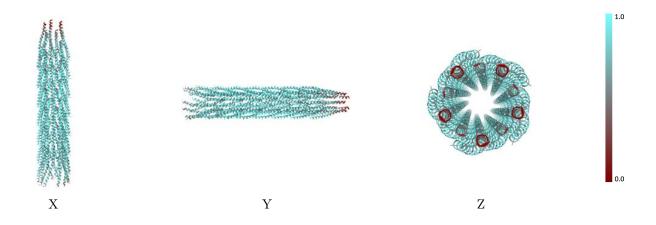


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

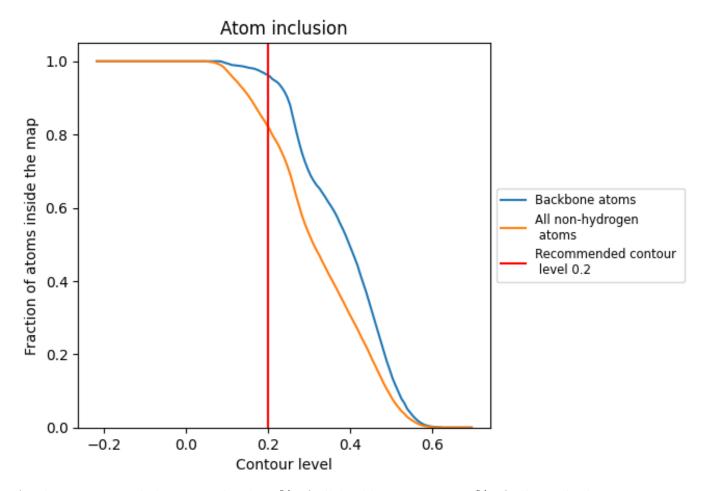
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).



9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.5510
AAA	0.8990	0.5740
AaA	0.8900	0.5750
AbA	0.8880	0.5660
AcA	0.8790	0.5620
AdA	0.8550	0.5530
AeA	0.8110	0.5420
AfA	0.7130	0.5280
AgA	0.7040	0.5220
AhA	0.8990	0.5710
AiA	0.8930	0.5710
AjA	0.8700	0.5610
AkA	0.8520	0.5570
AlA	0.7930	0.5420
AmA	0.7280	0.5280
AnA	0.6040	0.5100
BBB	0.8930	0.5730
BaB	0.8930	0.5720
BbB	0.8900	0.5690
BcB	0.8820	0.5630
BdB	0.8550	0.5540
BeB	0.8110	0.5400
BfB	0.7130	0.5230
BgB	0.7040	0.5220
BhB	0.8990	0.5690
BiB	0.8900	0.5700
BjB	0.8760	0.5640
BkB	0.8490	0.5550
BlB	0.7870	0.5400
BmB	0.7190	0.5310
BnB	0.5950	0.5120
CCC	0.8930	0.5720
CaC	0.8900	0.5700
CbC	0.8930	0.5700
CcC	0.8880	0.5640



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Chain	Atom inclusion	Q-score
CdC	0.8670	0.5540
CeC	0.8080	0.5410
CfC	0.7220	0.5240
CgC	0.7120	0.5200
ChC	0.8990	0.5690
CiC	0.8900	0.5670
CjC	0.8730	0.5620
CkC	0.8520	0.5560
ClC	0.7930	0.5440
CmC	0.7250	0.5310
CnC	0.5950	0.5140
DDD	0.8960	0.5710
DaD	0.8900	0.5690
DbD	0.8900	0.5680
DcD	0.8850	0.5610
DdD	0.8730	0.5540
DeD	0.8110	0.5450
DfD	0.7190	0.5260
DgD	0.7200	0.5230
DhD	0.8900	0.5690
DiD	0.8900	0.5680
DjD	0.8670	0.5630
DkD	0.8520	0.5570
DlD	0.7900	0.5460
DmD	0.7160	0.5310
DnD	0.6010	0.5110
EEE	0.8960	0.5720
EaE	0.8960	0.5700
EbE	0.8850	0.5670
EcE	0.8820	0.5630
EdE	0.8610	0.5550
EeE	0.7990	0.5410
EfE	0.7250	0.5260
EgE	0.7040	0.5250
EhE	0.8930	0.5720
EiE	0.8880	0.5670
EjE	0.8760	0.5640
EkE	0.8460	0.5570
ElE	0.7840	0.5430
EmE	0.7190	0.5290
EnE	0.5950	0.5100

