

Full wwPDB EM Validation Report (i)

Jul 29, 2024 – 04:35 PM EDT

PDB ID : 9CGM

EMDB ID : EMD-45583

Title : The Structure of Spiroplasma Virus 4

Authors: Mietzsch, M.; McKenna, R.

Deposited on : 2024-06-30

Resolution : 2.52 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.dev92

MolProbity : 4.02b-467

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

 $MapQ \quad : \quad 1.9.13$

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

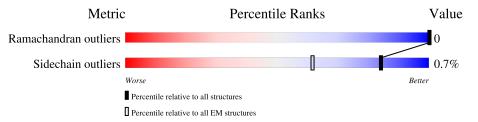
Validation Pipeline (wwPDB-VP) : 2.37.1

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 2.52 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	1	553	87%	13%
1	2	553	87%	13%
1	3	553	87%	13%
1	4	553	87%	13%
1	5	553	87%	13%
1	6	553	87%	13%
1	7	553	87%	13%
1	8	553	87%	13%
1	A	553	87%	13%



Mol	Chain	$oxed{ f Length }$	Quality of chain	
MIOI	Chain	Length	Quanty of chain	
1	В	553	87%	13%
1	С	553	87%	13%
1	D	553	87%	13%
1	Е	553	87%	13%
1	F	553	87%	13%
1	G	553	87%	13%
1	Н	553	87%	13%
1	I	553	87%	13%
1	J	553	<u> </u>	13%
1	K	553	<u>•</u>	
			87% ·	13%
1	L	553	87% ·	13%
1	M	553	87% ·	13%
1	N	553	87% ·	13%
1	О	553	87%	13%
1	Р	553	87%	13%
1	Q	553	87%	13%
1	R	553	87%	13%
1	S	553	87%	13%
1	Т	553	87%	13%
1	U	553	87%	13%
1	V	553	87%	13%
1	W	553	**************************************	13%
1	X	553	87%	13%
1	Y	553	87%	13%
1	Z	553	87%	13%
1		555	01/0	17 /0



Mol	Chain	Length	Quality of chain	
1	a	553	87%	13%
1	b	553	87%	13%
			<u>.</u>	
1	С	553	87% ·	13%
1	d	553	87% ·	13%
1	e	553	87%	13%
1	f	553	87%	13%
1	g	553	87%	13%
1	h	553	87%	13%
1	i	553	87%	13%
1	j	553	87%	13%
1	k	553	•	
			87% ·	13%
1	1	553	87% ·	13%
1	m	553	87% ·	13%
1	n	553	87%	13%
1	0	553	87%	13%
1	p	553	87%	13%
1	q	553	87%	13%
1	r	553	87%	13%
1	s	553	87%	13%
1		553	<u>.</u>	
	t		87% ·	13%
1	u	553	87% ·	13%
1	V	553	87%	13%
1	W	553	87%	13%
1	X	553	87%	13%
1	у	553	87%	13%



Mol	Chain	Length							
			•						
1	Z	553	87% 8%	• 13%					
2	0	38	79%	21%					
-	10	20	8%						
2	12	38	79% 8%	21%					
2	22	38	79%	21%					
0	20	20	8%						
2	32	38	79%	21%					
2	42	38	79%	21%					
2	52	38	8%	210/					
	32	30	79% 8%	21%					
2	62	38	79%	21%					
2	72	38	79%	21%					
	12	30	8%	21%					
2	82	38	79%	21%					
2	9	38	79%	21%					
			8%	2170					
2	C2	38	79%	21%					
2	D2	38	79%	21%					
			8%						
2	E2	38	79% 8%	21%					
2	F2	38	79%	21%					
0	CO	20	8%						
2	G2	38	79%	21%					
2	H2	38	79%	21%					
2	I2	38	8%						
	12	30	79% 8%	21%					
2	J2	38	79%	21%					
2	K2	38	8%	210/					
	11.2	30	79% 	21%					
2	L2	38	79%	21%					
2	M2	38	79%	21%					
			8%	Z I /0					
2	N2	38	79%	21%					
2	O2	38	79%	21%					
			8%	£170					
2	P2	38	79%	21%					



Mol	Chain	$oxed{ egin{array}{c} {f Length} \end{array} }$	Quality of chain	
			8%	
2	Q2	38	79%	21%
2	R2	38	79%	21%
2	S2	38	79%	21%
			8%	21%
2	T2	38	79%	21%
2	U2	38	79%	21%
2	V2	38	79%	21%
			8%	
2	W2	38	79% 	21%
2	X2	38	79%	21%
2	Y2	38	79%	21%
2	Z2	38	79%	21%
			8%	2170
2	a2	38	79% 8%	21%
2	b2	38	79%	21%
2	c2	38	79%	21%
2	d2	38	8%	
			79%	21%
2	e2	38	79%	21%
2	f2	38	79%	21%
2	g2	38	79%	21%
			8%	
2	h2	38	79%	21%
2	i2	38	79% 8%	21%
2	j2	38	79%	21%
2	k2	38	79%	21%
			8%	
2	12	38	79% 8%	21%
2	m2	38	79%	21%
2	n2	38	79%	21%
			8%	
2	02	38	79%	21%



Mol	Chain	Length	Quality of ch	ain
2	p2	38	79%	21%
2	q2	38	79%	21%
2	r2	38	79% 8%	21%
2	s2	38	79%	21%
2	t2	38	79%	21%
2	u2	38	79% 8%	21%
2	v2	38	79%	21%
2	w2	38	79% 8%	21%
2	x2	38	79% 8%	21%
2	y2	38	79% 8%	21%
2	z2	38	79%	21%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 246420 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 VP1.

Mol	Chain	Residues		At	oms			AltConf	Trace														
1	Λ	400	Total	С	N	О	S	0	0														
1	A	482	3853	2458	665	716	14	0	0														
1	D	400	Total	С	N	О	S	0	0														
1	В	482	3853	2458	665	716	14	0	0														
1	С	499	Total	С	N	О	S	0	0														
1	C	482	3853	2458	665	716	14	U	0														
1	D	482	Total	С	N	О	S	0	0														
1	D		3853	2458	665	716	14	U	0														
1		199	Total	С	N	О	S	0	0														
1	\mathbf{E}	482	3853	2458	665	716	14	U	U														
1	F	482	Total	С	N	О	S	0	0														
1	Г	402	3853	2458	665	716	14		U														
1	G	482	Total	С	N	О	S	0	0														
1	G	402	3853	2458	665	716	14	U															
1	Н	482	Total	С	N	О	S	0	0														
1	11	402	3853	2458	665	716	14	U	0														
1	I	482	Total	С	N	О	S	0	0														
1	1	402	3853	2458	665	716	14	U	0														
1	J	482	Total	С	N	O	S	0	0														
1	J	402	3853	2458	665	716	14	0															
1	K	482	Total	\mathbf{C}	N	O	\mathbf{S}	0	0														
1	11	402	3853	2458	665	716	14	U	U														
1	L	482	Total	С	N	O	\mathbf{S}	0	0														
1	П	402	3853	2458	665	716	14	U	U														
1	M	482	Total	\mathbf{C}	N	O	\mathbf{S}	0	0														
1	1V1	402	3853	2458	665	716	14	O	U														
1	N	482	Total	С	Ν	О	S	0	0														
1	11	402	3853	2458	665	716	14	O	U														
1	О	482	Total	С	N	О	\mathbf{S}	0	0														
1		102	3853	2458	665	716	14	U	0														
1	Р	482	Total	С	N	О	\mathbf{S}	0	0														
1		102	3853	2458	665	716	14	U	U														
1	Q	482	Total	С	N	O	\mathbf{S}	0	0														
		Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	-104	3853	2458	665	716	14	1 0



Mol	Chain	$oxed{ egin{array}{c} \mathbf{Residues} \end{array} }$	<i>ye</i>	A t.	oms		AltConf	Trace	
IVIOI	Cilain	residues	Total	$\frac{110}{C}$	N	0	S	7110COIII	Trace
1	R	482	3853	2458	665	716	14	0	0
	~	400	Total	C	N	0	S		
1	S	482	3853	2458	665	716	14	0	0
1	Т	400	Total	С	N	О	S	0	0
1	1	482	3853	2458	665	716	14	0	0
1	U	482	Total	С	N	О	S	0	0
1	U	402	3853	2458	665	716	14	U	U
1	V	482	Total	С	Ν	Ο	S	0	0
1	V	402	3853	2458	665	716	14	U	U
1	W	482	Total	\mathbf{C}	N	Ο	S	0	0
1	***	402	3853	2458	665	716	14	U	
1	X	482	Total	\mathbf{C}	N	O	S	0	0
1	21	102	3853	2458	665	716	14	Ů,	0
1	Y	482	Total	\mathbf{C}	N	Ο	S	0	0
	1	102	3853	2458	665	716	14		
1	Z	482	Total	С	N	О	S	0	0
		102	3853	2458	665	716	14		
1	a	482	Total	С	N	Ο	S	0	0
	a	402	3853	2458	665	716	14		
1	b	482	Total	\mathbf{C}	N	О	S	0	0
	~	102	3853	2458	665	716	14	U	
1	c	482	Total	С	N	Ο	S	0	0
1	0	102	3853	2458	665	716	14		
1	d	482	Total	С	N	Ο	S	0	0
	u u	102	3853	2458	665	716	14	<u> </u>	0
1	e	482	Total	С	N	Ο	S	0	0
	- C	102	3853	2458	665	716	14	Ŭ	
1	f	482	Total	С	N	О	S	0	0
	-	102	3853	2458	665	716	14	Ŭ	Ů
1	g	482	Total	\mathbf{C}	N	О	S	0	0
	8	102	3853	2458	665	716	14		
1	h	482	Total	\mathbf{C}	N	О	S	0	0
_		-0-	3853	2458	665	716	14		
1	i	482	Total	С	N	O	S	0	0
_	_		3853	2458	665	716	14		Ŭ,
1	i	j 482	Total	C	N	0	S	0	0
_	J		3853	2458	665	716	14		
1	k	482	Total	C	N	0	S	0	0
_			3853	2458	665	716	14		
1	1 l	482	Total	C	N	0	S	0	0
		_	3853	2458	665	716	14	U	U



1 m 482 Total Sassa 2458 665 716 14 2 0 0 0 0	Mol	Chain	Residues	<i>g</i> =	At	oms			AltConf	Trace
1	-1		400	Total	С	N	О	S	0	0
1 n 482 3853 2458 665 716 14 0 0 1 o 482 Total C N O S 1 p 482 Total C N O S 1 p 482 Total C N O S 1 q 482 Total C N O S 1 r 482 Total C N O S 1 r 482 Total C N O S 1 r 482 Total C N O S 1 t 482 Total C N O S 1 t 482 3853 2458 665 716 14 O O 1 u 482 3853 2458 665 716 14 <t< td=""><td>1</td><td>m</td><td>482</td><td></td><td>2458</td><td>665</td><td>716</td><td>14</td><td>0</td><td>0</td></t<>	1	m	482		2458	665	716	14	0	0
1	-1		400	Total	С	N	О	S	0	0
1 0 482 3853 2458 665 716 14 0 0 1 p 482 Total C N O S 0 0 1 q 482 Total C N O S 0 0 1 r 482 Total C N O S 0 0 1 r 482 Total C N O S 0 0 1 s 482 Total C N O S 0 0 1 t 482 Total C N O S 0 0 1 u 482 Total C N O S 0 0 1 u 482 Total C N O S 0 0 1 w 482 Total <th< td=""><td>1</td><td>n</td><td>482</td><td>3853</td><td>2458</td><td>665</td><td>716</td><td>14</td><td>0</td><td>U</td></th<>	1	n	482	3853	2458	665	716	14	0	U
1 p 482 Total C N O S S SS53 2458 665 716 14 0 0 1 q 482 Total C N O S S S SS53 2458 665 716 14 0 0 1 q 482 Total C N O S S S SS53 2458 665 716 14 0 0 1 r 482 3853 2458 665 716 14 0 0 1 s 482 3853 2458 665 716 14 0 0 1 s 482 3853 2458 665 716 14 0 0 1 t 482 3853 2458 665 716 14 0 0 1 u 482 3853 2458 665 716 14 0 0 1 u 482 3853 2458 665 716 14 0 0 1 w 482 3853 2458 665 716 14 0 0 1 w 482 3853 2458 665 716 14 0 0 1 w 482 3853 2458 665 716 14 0 0 1 x 482 3853 2458 665 716 14 0 0	1		400	Total	С	N	О	S	0	0
1 p 482 3853 2458 665 716 14 0 0 1 q 482 Total C N O S 0 0 1 r 482 Total C N O S 0 0 1 s 482 Total C N O S 0 0 1 s 482 Total C N O S 0 0 1 t 482 Total C N O S 0 0 0 1 u 482 Total C N O S 0 0 0 1 v 482 Total C N O S 0 0 0 1 v 482 Total C N O S 0 0 0 1 <td>1</td> <td>O</td> <td>482</td> <td>3853</td> <td>2458</td> <td>665</td> <td>716</td> <td>14</td> <td>0</td> <td>U</td>	1	O	482	3853	2458	665	716	14	0	U
1 q 482 Total C N O S S 3853 2458 665 716 14 0 0 1 r 482 Total C N O S 3853 2458 665 716 14 0 0 1 r 482 Total C N O S 3853 2458 665 716 14 0 0 1 s 482 Total C N O S 3853 2458 665 716 14 0 0 1 t 482 Total C N O S 3853 2458 665 716 14 0 0 1 u 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0	1		400	Total	С	N	О	S	0	0
1 q 482 3853 2458 665 716 14 0 0 1 r 482 Total C N O S 0 0 1 s 482 Total C N O S 0 0 1 t 482 Total C N O S 0 0 1 t 482 Total C N O S 0 0 1 u 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 w 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 y 482 Total	1	p	482	3853	2458	665	716	14	0	U
1 r 482 Total C N O S 3853 2458 665 716 14 0 0 1 s 482 Total C N O S 3853 2458 665 716 14 0 0 1 s 482 Total C N O S 3853 2458 665 716 14 0 0 1 t 482 Total C N O S 3853 2458 665 716 14 0 0 1 u 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 <t< td=""><td>1</td><td></td><td>400</td><td>Total</td><td>С</td><td>N</td><td>О</td><td>S</td><td>0</td><td>0</td></t<>	1		400	Total	С	N	О	S	0	0
1 r 482 3853 2458 665 716 14 0 0 1 s 482 Total C N O S 0 0 1 t 482 Total C N O S 0 0 1 u 482 Total C N O S 0 0 1 u 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 w 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 x 482 Total	1	q	482	3853	2458	665	716	14	U	U
1 s 482 Total C N O S 3853 2458 665 716 14 0 0 1 t 482 Total C N O S 3853 2458 665 716 14 0 0 1 t 482 Total C N O S 3853 2458 665 716 14 0 0 1 u 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 <t< td=""><td>1</td><td></td><td>400</td><td>Total</td><td>С</td><td>N</td><td>О</td><td>S</td><td>0</td><td>0</td></t<>	1		400	Total	С	N	О	S	0	0
1 s 482 3853 2458 665 716 14 0 0 1 t 482 Total C N O S 0 0 1 u 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 w 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total	1	Γ	482	3853	2458	665	716	14	U	U
1 t 482 Total C N O S 3853 2458 665 716 14 0 0 1 u 482 Total C N O S 3853 2458 665 716 14 0 0 1 u 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 <t< td=""><td>1</td><td>G</td><td>499</td><td>Total</td><td>С</td><td>N</td><td>О</td><td>S</td><td>0</td><td>0</td></t<>	1	G	499	Total	С	N	О	S	0	0
1 t 482 3853 2458 665 716 14 0 0 1 u 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 v 482 Total C N O S 0 0 1 w 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total	1	S	402	3853	2458	665	716	14	U	0
1 u 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 <t< td=""><td>1</td><td>4</td><td rowspan="2">482</td><td>Total</td><td>С</td><td>N</td><td>О</td><td>S</td><td>0</td><td rowspan="2">0</td></t<>	1	4	482	Total	С	N	О	S	0	0
1 u 482 3853 2458 665 716 14 0 0 1 v 482 Total C N O S 0 0 1 w 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 y 482 Total	1	l t		3853	2458	665	716	14	U	
1 v 482 Total C N O S 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 3853 2458 665 716 14 0 0 1 1 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 <t< td=""><td>1</td><td></td><td>400</td><td>Total</td><td>С</td><td>N</td><td>О</td><td>S</td><td>0</td><td></td></t<>	1		400	Total	С	N	О	S	0	
1 v 482 3853 2458 665 716 14 0 0 1 w 482 Total C N O S 0 0 1 x 482 Total C N O S 0 0 1 y 482 3853 2458 665 716 14 0 0 1 y 482 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 0 0 1 482 Total C N O S 0 0 0 1 2 482 Total C N O S 0 0 0 1 3 482 Total C N O S 0 0 0 1 4 482 Total C N O S 0 0 0	1	u	482	3853	2458	665	716	14	U	U
1 w 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 3853 2458 665 716 14 0 0 1 1 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 <t< td=""><td>1</td><td></td><td rowspan="2">482</td><td>Total</td><td>С</td><td>N</td><td>О</td><td>S</td><td>0</td><td></td></t<>	1		482	Total	С	N	О	S	0	
1 w 482 3853 2458 665 716 14 0 0 1 x 482 Total C N O S 0 0 1 y 482 Total C N O S 0 0 1 z 482 Total C N O S 0 0 1 1 482 Total C N O S 0 0 1 1 482 Total C N O S 0 0 1 2 482 Total C N O S 0 0 1 3 482 Total C N O S 0 0 1 4 482 Total C N O S 0 0 1 4 482 Total C N O S 0 0 1 482 Total C	1	V		3853	2458	665	716	14	U	U
1 x 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 3853 2458 665 716 14 0 0 1 1 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 3853 2458 665 716 14 0 0	1		482	Total	С	N	О	S	0	0
1 x 482 3853 2458 665 716 14 0 0 1 y 482 Total C N O S 0 0 1 z 482 Total C N O S 0 0 1 1 482 Total C N O S 0 0 1 2 482 Total C N O S 0 0 1 3 482 Total C N O S 0 0 1 3 482 Total C N O S 0 0 1 4 482 Total C N O S 0 0 1 5 482 Total C N O S 0 0 1 6 482 Total C N O S 0 0 1 7 482 Total	1	W		3853	2458	665	716	14	U	
1 y 482 Total C N O S 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 3853 2458 665 716 14 0 0 1 1 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 716 14 0 0 1 7 482 Total C N O S 716 14 0 0 1 7 482 Total C N O S 716 14 0 0	1		499	Total	С	N	О	S	0	0
1 y 482 3853 2458 665 716 14 0 0 1 z 482 Total C N O S 0 0 1 1 482 Total C N O S 0 0 1 2 482 Total C N O S 0 0 1 3 482 Total C N O S 0 0 1 4 482 Total C N O S 0 0 1 4 482 Total C N O S 0 0 1 5 482 Total C N O S 0 0 1 6 482 Total C N O S 0 0 1 7 482 Total C N O S 0 0	1	X	402	3853	2458	665	716	14	0	
1 z 482 Total C N O S 3853 2458 665 716 14 0 0 1 1 482 Total C N O S 3853 2458 665 716 14 0 0 1 1 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 3853 2458 665 716 14 0 0	1		499	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	У	402	3853	2458	665	716	14	0	U
1 1 482 Total C N O S 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 716 14 0 0	1	-	189	Total	С	N	О	S	0	0
1 1 482 3853 2458 665 716 14 0 0 1 2 482 Total C N O S 0 0 1 3 482 Total C N O S 0 0 1 4 482 Total C N O S 0 0 1 5 482 Total C N O S 0 0 1 6 482 Total C N O S 0 0 1 7 482 Total C N O S 0 0 1 7 482 Total C N O S 0 0	1	Z	402	3853	2458	665	716	14	0	U
1 2 482 Total C N O S 3853 2458 665 716 14 0 0 1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 3853 2458 665 716 14 0 0	1	1	489	Total	С	N	О	S	0	0
1 2 482 3853 2458 665 716 14 0 0 1 3 482 Total 3853 C N O S 0 0 1 4 482 Total 3853 C N O S 0 0 1 5 482 Total 3853 C N O S 0 0 1 6 482 Total 3853 C N O S 0 0 1 7 482 Total Total Total C N O S 0 0	1	1	402	3853	2458	665	716	14	0	U
1 3 482 Total C N O S 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 3853 2458 665 716 14 0 0	1	2	189	Total	С	N	О	S	0	0
1 3 482 3853 2458 665 716 14 0 0 1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 716 14 0 0 1 7 482 Total C N O S 716 0 0	1	2	402	3853	2458	665	716		U	U
1 4 482 Total C N O S 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 3853 2458 665 716 14 0 0	1	3	189	Total	С	N	Ο	S	0	0
1 4 482 3853 2458 665 716 14 0 0 1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 0 0 0	1	3	402	3853	2458	665	716	14	0	U
1 5 482 Total C N O S 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 0 0 0	1	4	489			N	O	\overline{S}	0	0
1 5 482 3853 2458 665 716 14 0 0 1 6 482 Total C N O S 0 0 1 7 482 Total C N O S 0 0		4	402	3853			716		U	U
1 6 482 Total C N O S 0 0 1 7 482 Total C N O S 0 0	1	5 489						0	0	
1 6 482 3853 2458 665 716 14 0 0 1 7 482 Total C N O S 0	1	3	5 482						U	0
1 7 482 Total C N O S 0 0	1	6 489					\mathbf{S}	0	0	
1 + 7 + 489 + 0 + 0 + 0 + 0	1	J	102						U	0
3853 2458 665 716 14	1	7	482						0	0
Continued on next mase		'	102	3853	2458	665	716	14		



Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	482	Total 3853	C 2458	N 665	O 716	S 14	0	0

• Molecule 2 is a protein called DNA binding protein ORF8.

Mol	Chain	Residues		Ato	ms			AltConf	Trace
0	0	20	Total	С	N	О	S	0	0
2	0	30	254	155	61	37	1	0	0
2	9	30	Total	С	N	О	S	0	0
<u></u>	9	30	254	155	61	37	1	0	U
2	C2	30	Total	С	N	О	S	0	0
<u> </u>	02	30	254	155	61	37	1	0	U
2	D2	30	Total	С	N	Ο	S	0	0
2	102	30	254	155	61	37	1	0	O
2	E2	30	Total	С	N	Ο	S	0	0
	177	30	254	155	61	37	1	U	U
2	F2	30	Total	\mathbf{C}	N	Ο	S	0	0
	1.7	30	254	155	61	37	1	U	U
2	G2	30	Total	С	N	Ο	S	0	0
	0.2	30	254	155	61	37	1	Ü	<u> </u>
2	H2	30	Total	С	N	Ο	S	0	0
	112	90	254	155	61	37	1		
2	I2	30	Total	С	N	О	S	0	0
	12	30	254	155	61	37	1		
2	J2	30	Total	С	N	O	S	0	0
			254	155	61	37	1		
2	K2	30	Total	С	N	0	S	0	0
			254	155	61	37	1	_	
2	L2	30	Total	С	N	0	S	0	0
			254	155	61	37	1		
2	M2	30	Total	С	N	0	S	0	0
			254	155	61	37	1		
2	N2	30	Total	C	N	0	S	0	0
			254	155	61	37	1		
2	O2	30	Total	C	N	0	S	0	0
			254	155	61	37	1		
2	P2	30	Total	C	N c1	0	S	0	0
			254	$\frac{155}{C}$	61 N	37	$\frac{1}{\mathbf{c}}$		
2	Q2	30	Total	C	N 61	0	S	0	0
			254	$\frac{155}{C}$	61 N	37	$\frac{1}{\mathbf{c}}$		
2	R2	30	Total		N 61	O 27	S	0	0
	n2		254	155	61	37	1		



Mol	Chain	$oxed{ \mathbf{Residues} }$	Atoms				AltConf	Trace	
2	CO	30	Total	С	N	О	S	0	0
	S2		254	155	61	37	1	0	0
2	ТО	30	Total	С	N	О	S	0	0
	T2		254	155	61	37	1		
2	U2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	V2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	W2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	X2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	Y2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	Z2	30	Total	С	N	О	S	0	0
	212		254	155	61	37	1		
2	a2	30	Total	С	Ν	Ο	S	0	0
	a2		254	155	61	37	1	O	
2	b2	30	Total	С	N	Ο	S	0	0
	2 02		254	155	61	37	1		
2	c2	30	Total	С	N	Ο	S	0	0
	02		254	155	61	37	1		
2	d2	30	Total	С	N	О	S	0	0
	G.2		254	155	61	37	1		
$\frac{1}{2}$	e2	30	Total	С	N	Ο	S	0	0
			254	155	61	37	1		
2	f2	30	Total	С	N	Ο	S	0	0
			254	155	61	37	1		
2	g2	30	Total	С	N	O	S	0	0
_	0-		254	155	61	37	1		
2	h2	30	Total	С	N	O	S	0	0
_			254	155	61	37	1		
2	i2	30	Total	С	N	O	S	0	0
			254	155	61	37	1		
2	j2	30	Total	C	N	0	S	0	0
		-	254	155	61	37	1	-	
2	k2	30	Total	C	N	0	S	0	0
			254	155	61	37	$\frac{1}{C}$		
			Total	С	N	0	S		
			254	155	61	37	$\frac{1}{C}$		
2	m2	30	Total	C	N	0	S	0	0
			254	155	61	37	1		

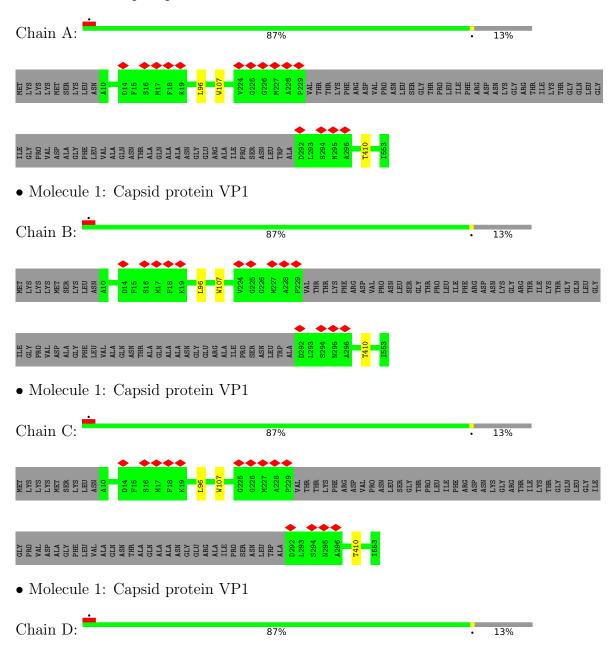


Mol	Chain	Residues	<i>3</i> - · · ·	Ato	ms			AltConf	Trace
2	0	30	Total						0
	n2		254	155	61	37	1	0	0
2	-	30	Total	С	N	О	S	0	0
	02		254	155	61	37	1		
2	p2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	q2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	r2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	s2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	t2	30	Total	С	N	О	S	0	0
<u> </u>			254	155	61	37	1		
2	u2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	v2	30	Total	С	N	Ο	S	0	0
	V 2		254	155	61	37	1	0	
2	w2	30	Total	С	Ν	Ο	S	0	0
	VV Z		254	155	61	37	1		
2	x2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	y2	30	Total	С	N	О	S	0	0
			254	155	61	37	1		
2	z2	30	Total	С	N	Ο	S	0	0
			254	155	61	37	1		
2	12	30	Total	С	N	O	S	0	0
			254	155	61	37	1		
2	22	30	Total	С	N	0	S	0	0
_			254	155	61	37	1		
2	32	30	Total	С	N	0	S	0	0
			254	155	61	37	1		
2	42	30	Total	С	N	0	S	0	0
			254	155	61	37	1		
2	52	30	Total	C	N	0	S	0	0
			254	155	61	37	1		
2	62 72	30	Total	C	N	0	S	0	0
			254	$\frac{155}{C}$	61 N	37	1		
2			Total	C	N	0	S		
2	82	30	254	155 C	61 N	37	$\frac{1}{C}$	0	0
			Total	C	N 61	0	S		
			254	155	61	37	1		



3 Residue-property plots (i)

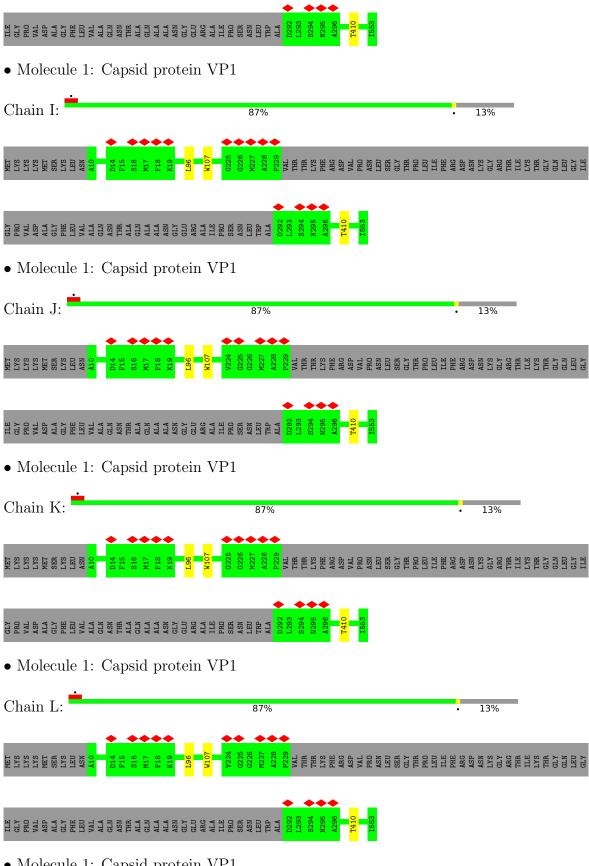
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.



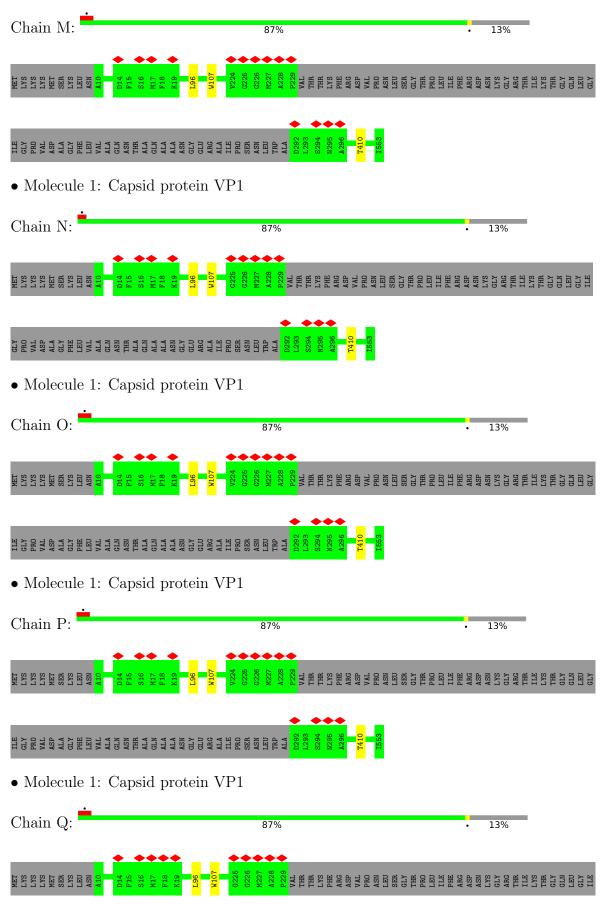




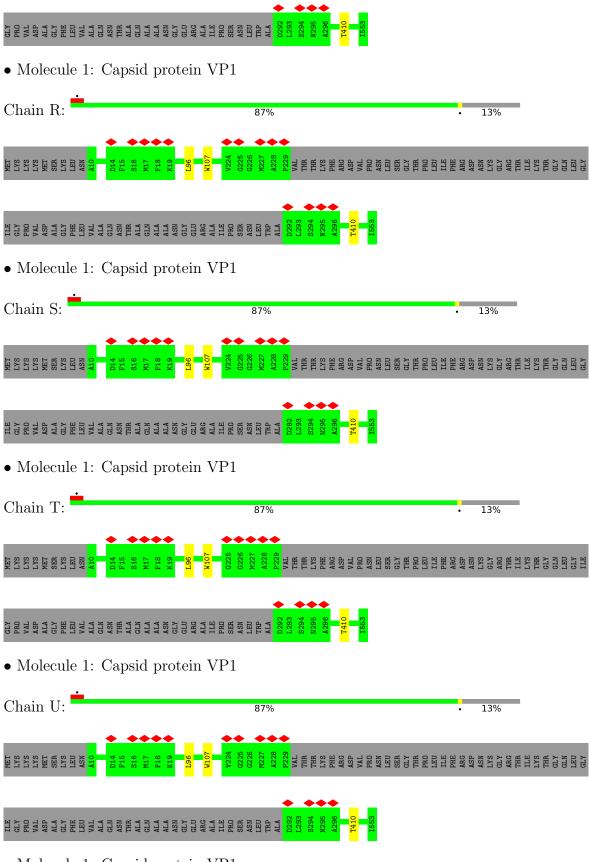




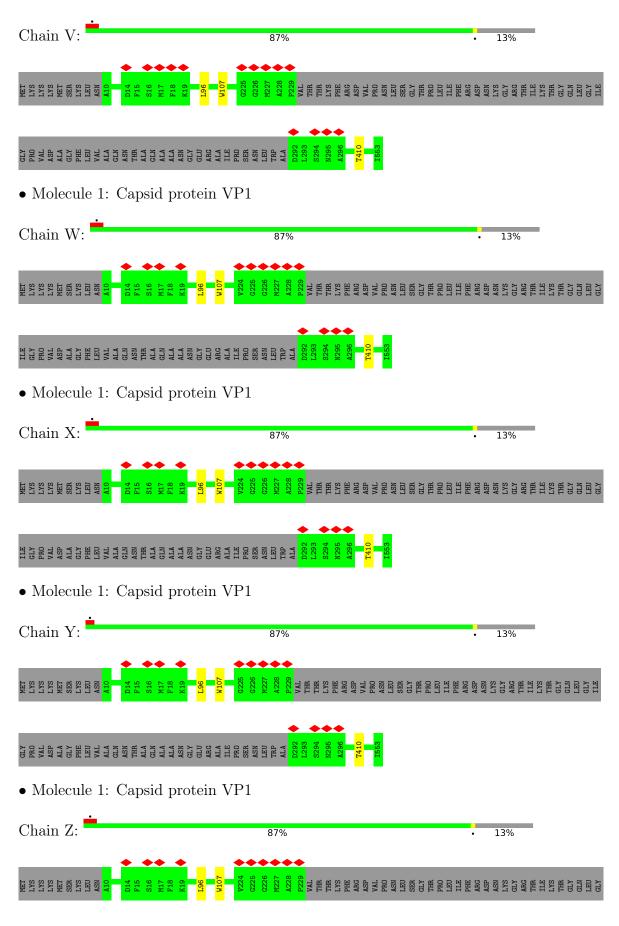




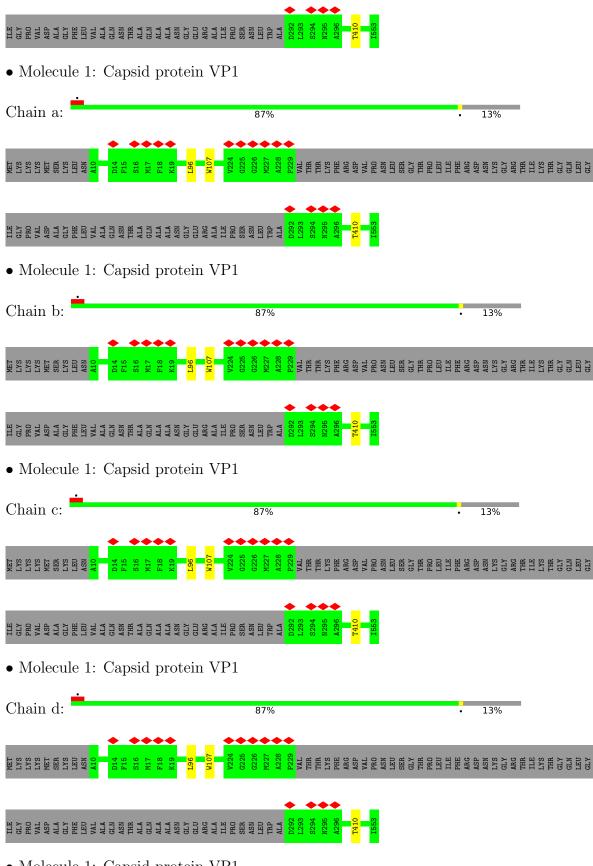




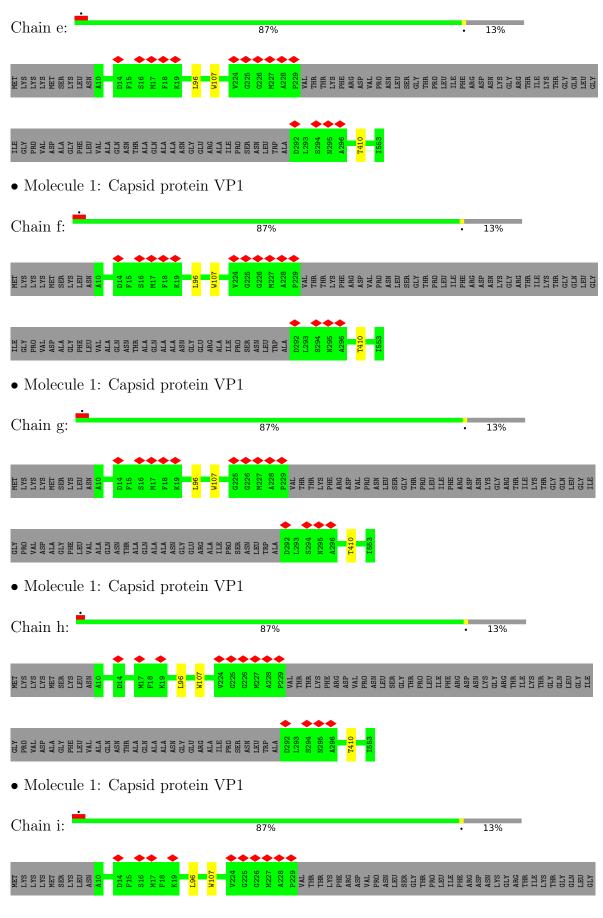




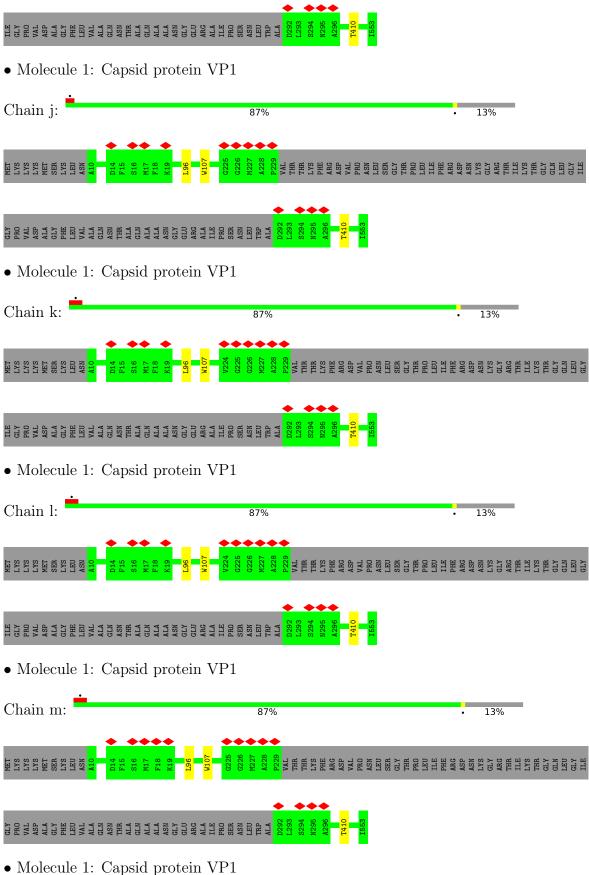




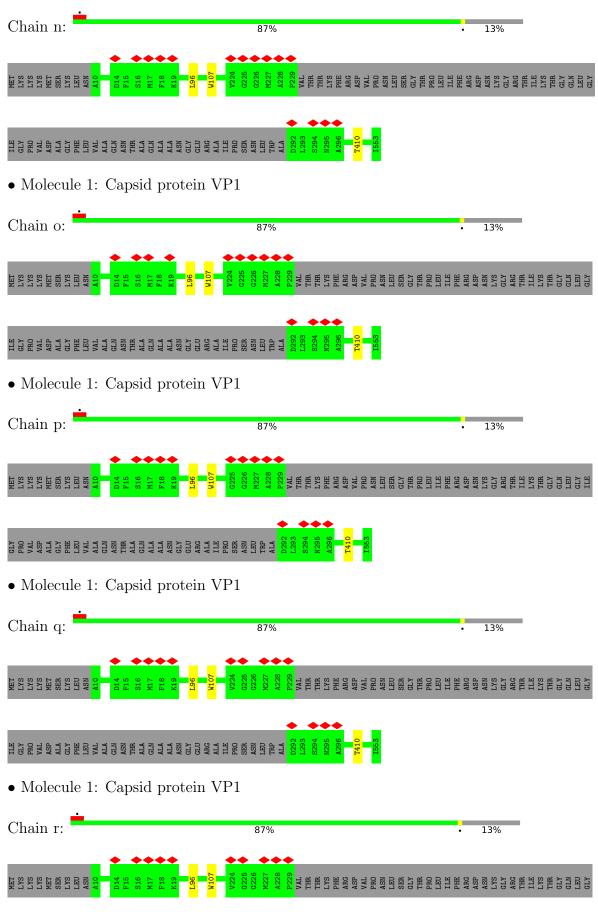




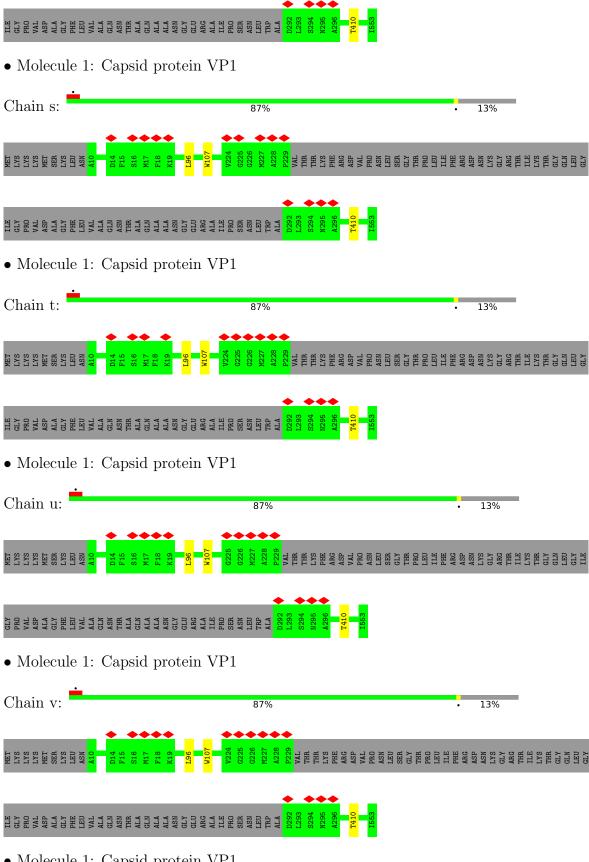




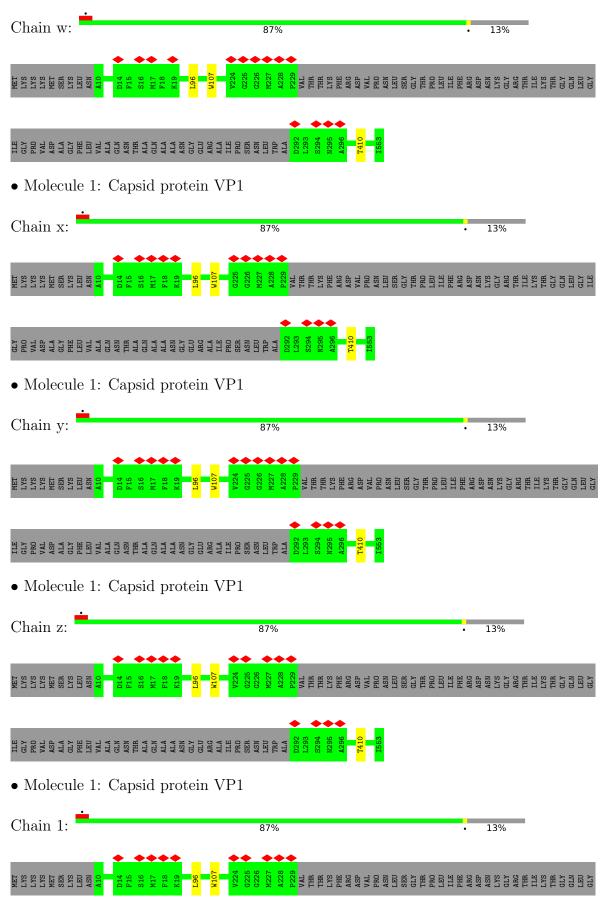




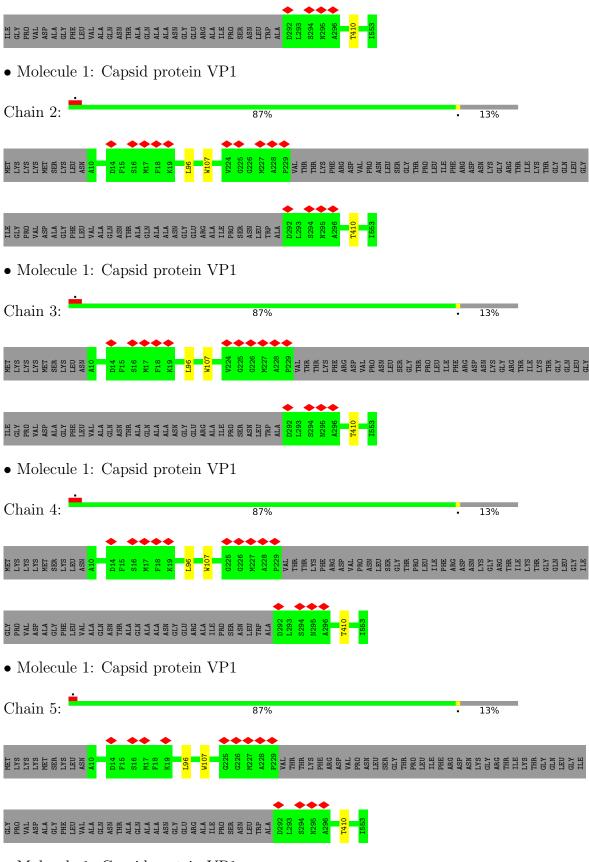




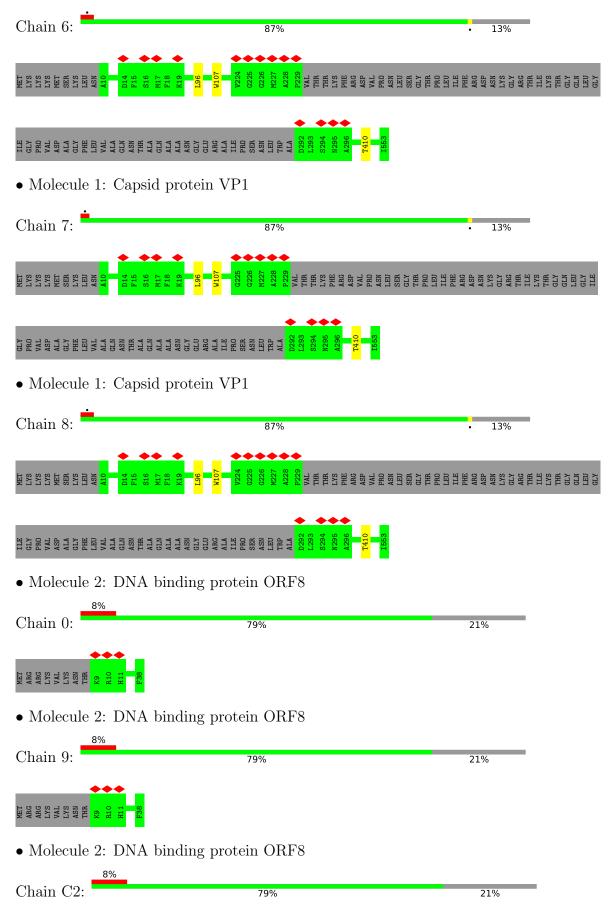








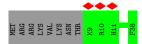






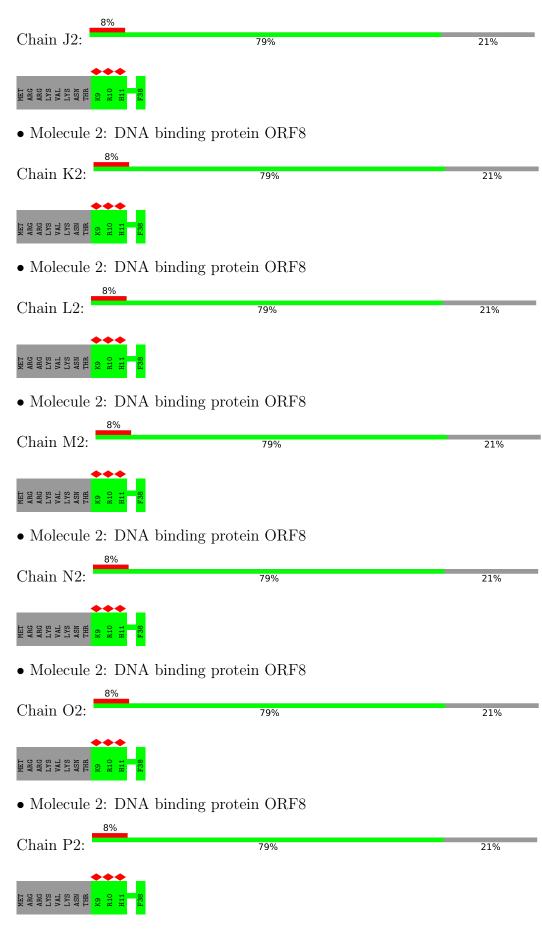


Chain I2: 79% 21%

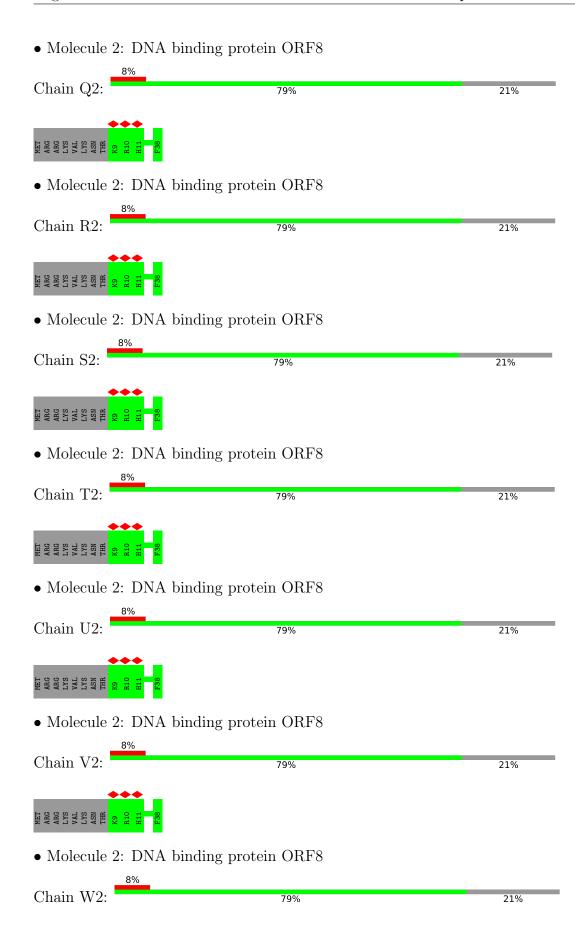


• Molecule 2: DNA binding protein ORF8

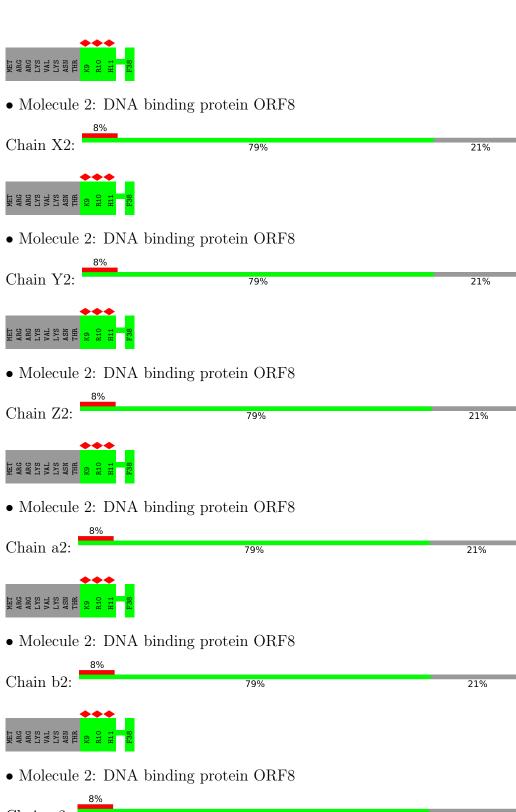




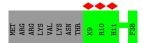








Chain c2: 21%

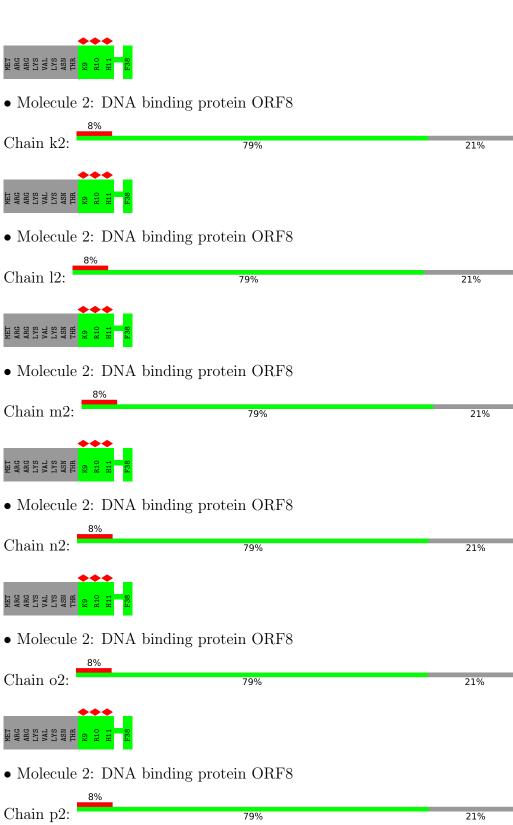


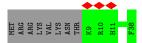
• Molecule 2: DNA binding protein ORF8











• Molecule 2: DNA binding protein ORF8

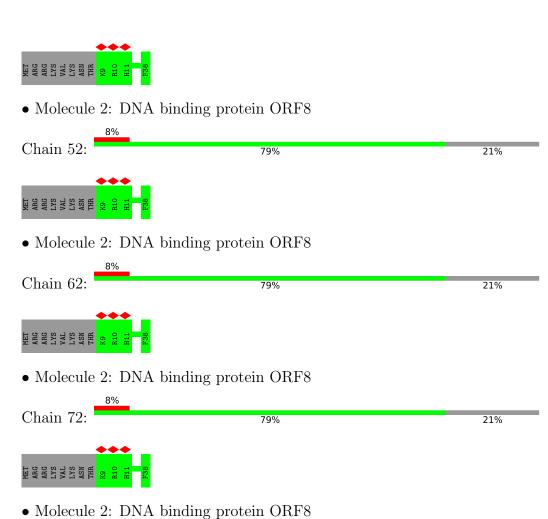












79%



22/





21%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	77204	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.707	Depositor
Minimum map value	-14.782	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	583.55, 583.55, 583.55	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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	langles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	1	0.46	0/3961	0.54	0/5385
1	2	0.46	0/3961	0.54	0/5385
1	3	0.46	0/3961	0.54	0/5385
1	4	0.46	0/3961	0.54	0/5385
1	5	0.46	0/3961	0.54	0/5385
1	6	0.46	0/3961	0.54	0/5385
1	7	0.46	0/3961	0.54	0/5385
1	8	0.46	0/3961	0.54	0/5385
1	A	0.46	0/3961	0.54	0/5385
1	В	0.46	0/3961	0.54	0/5385
1	С	0.46	0/3961	0.54	0/5385
1	D	0.46	0/3961	0.54	0/5385
1	Е	0.46	0/3961	0.54	0/5385
1	F	0.46	0/3961	0.54	0/5385
1	G	0.46	0/3961	0.54	0/5385
1	Н	0.46	0/3961	0.54	0/5385
1	I	0.45	0/3961	0.54	0/5385
1	J	0.46	0/3961	0.54	0/5385
1	K	0.46	0/3961	0.54	0/5385
1	L	0.46	0/3961	0.54	0/5385
1	M	0.46	0/3961	0.54	0/5385
1	N	0.46	0/3961	0.54	0/5385
1	О	0.46	0/3961	0.54	0/5385
1	Р	0.46	0/3961	0.54	0/5385
1	Q	0.46	0/3961	0.54	0/5385
1	R	0.46	0/3961	0.54	0/5385
1	S	0.46	0/3961	0.54	0/5385
1	Т	0.46	0/3961	0.54	0/5385
1	U	0.46	0/3961	0.54	0/5385
1	V	0.46	0/3961	0.54	0/5385
1	W	0.46	0/3961	0.54	0/5385
1	X	0.46	0/3961	0.54	0/5385
1	Y	0.46	0/3961	0.54	0/5385
1	Z	0.46	0/3961	0.54	0/5385



		Rond	longths	Pond	Bond angles		
Mol	Chain	RMSZ	lengths $ \# Z > 5$	RMSZ			
1	_				# Z > 5		
1	a	0.46	0/3961	0.54	0/5385		
1	b	0.46	0/3961	0.54	0/5385		
1	С	0.46	0/3961	0.54	0/5385		
1	d	0.46	0/3961	0.54	0/5385		
1	е	0.46	0/3961	0.54	0/5385		
1	f	0.46	0/3961	0.54	0/5385		
1	g	0.46	0/3961	0.54	0/5385		
1	h	0.46	0/3961	0.54	0/5385		
1	i	0.46	0/3961	0.54	0/5385		
1	j	0.46	0/3961	0.54	0/5385		
1	k	0.46	0/3961	0.54	0/5385		
1	1	0.46	0/3961	0.54	0/5385		
1	m	0.46	0/3961	0.54	0/5385		
1	n	0.46	0/3961	0.54	0/5385		
1	О	0.46	0/3961	0.54	0/5385		
1	р	0.46	0/3961	0.54	0/5385		
1	q	0.46	0/3961	0.54	0/5385		
1	r	0.46	0/3961	0.54	0/5385		
1	S	0.46	0/3961	0.54	0/5385		
1	t	0.46	0/3961	0.54	0/5385		
1	u	0.46	0/3961	0.54	0/5385		
1	V	0.46	0/3961	0.54	0/5385		
1	W	0.46	0/3961	0.54	0/5385		
1	X	0.46	0/3961	0.54	0/5385		
1	y	0.46	0/3961	0.54	0/5385		
1	Z	0.46	0/3961	0.54	0/5385		
2	0	0.38	0/260	0.57	0/345		
2	12	0.38	0/260	0.57	0/345		
2	22	0.38	0/260	0.57	0/345		
2	32	0.38	0/260	0.58	0/345		
$\frac{2}{2}$	42	0.38	0/260	0.57	0/345		
2	52	0.38	0/260	0.58	0/345		
2	62	0.38	0/260	0.57	0/345		
2	72	0.38	0/260	0.57	0/345		
2	82	0.37	0/260	0.58	0/345 $0/345$		
$\frac{2}{2}$	9	0.38	0/260	0.57	0/345		
$\frac{2}{2}$	C2	0.38	0/260	0.57	0/345		
$\frac{2}{2}$	D2	0.38	0/260	0.57	0/345		
$\frac{2}{2}$	E2	0.38	0/260	0.57	0/345 $0/345$		
$\frac{2}{2}$	F2	0.38	0/260	0.57	0/345 $0/345$		
2	$\frac{\text{F2}}{\text{G2}}$	0.38	0/260	0.57	0/345 $0/345$		
$\frac{2}{2}$	H2		0/260		/		
		0.38	,	0.58	0/345		
2	I2	0.38	0/260	0.57	0/345		



		Rond	lengths	engths Bond ang		
Mol	Chain	RMSZ	# Z >5	RMSZ	$\mid \# Z > 5$	
2	J2	0.38	0/260	0.57	$\frac{\# Z >5}{0/345}$	
$\frac{2}{2}$	K2	0.38	0/260	0.57	$\frac{0/345}{0/345}$	
$\frac{2}{2}$	L2	0.38	0/260	0.57	$\frac{0/345}{0/345}$	
2	M2	0.38	0/260	0.57	$\frac{0/345}{0/345}$	
$\frac{2}{2}$			1		/	
$\frac{2}{2}$	N2 O2	0.38	0/260	0.57	0/345	
$\frac{2}{2}$		0.38	0/260	0.57	0/345	
	P2	0.38	0/260	0.58	0/345	
2	Q2	0.38	0/260	0.57	0/345	
2	R2	0.38	0/260	0.57	0/345	
2	S2	0.38	0/260	0.57	0/345	
2	T2	0.38	0/260	0.57	0/345	
2	U2	0.37	0/260	0.57	0/345	
2	V2	0.38	0/260	0.57	0/345	
2	W2	0.38	0/260	0.58	0/345	
2	X2	0.38	0/260	0.57	0/345	
2	Y2	0.38	0/260	0.57	0/345	
2	Z2	0.38	0/260	0.57	0/345	
2	a2	0.38	0/260	0.57	0/345	
2	b2	0.38	0/260	0.58	0/345	
2	c2	0.38	0/260	0.58	0/345	
2	d2	0.38	0/260	0.57	0/345	
2	e2	0.38	0/260	0.57	0/345	
2	f2	0.38	0/260	0.58	0/345	
2	g2	0.38	0/260	0.57	0/345	
2	h2	0.38	0/260	0.57	0/345	
2	i2	0.38	0/260	0.57	0/345	
2	j2	0.38	0/260	0.58	0/345	
2	k2	0.38	0/260	0.57	0/345	
2	12	0.38	0/260	0.57	0/345	
2	m2	0.38	0/260	0.57	0/345	
2	n2	0.38	0/260	0.57	0/345	
2	о2	0.38	0/260	0.57	0/345	
2	p2	0.38	0/260	0.57	0/345	
2	q2	0.38	0/260	0.57	0/345	
2	r2	0.38	0/260	0.57	0/345	
2	s2	0.38	0/260	0.57	0/345	
2	t2	0.38	0/260	0.57	0/345	
2	u2	0.38	0/260	0.57	0/345	
2	v2	0.38	0/260	0.57	0/345	
2	w2	0.38	0/260	0.57	0/345	
2	x2	0.38	0/260	0.57	0/345	
2		0.38	0/260	0.57	0/345	
2	z2	0.37	0/260	0.58	0/345	
2 2	x2 y2	0.38 0.38	0/260 $0/260$	0.57 0.57	0/345 0/345	



Mal	Chain	Bond lengths		Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
All	All	0.45	0/253260	0.54	0/343800

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	Percer	ntiles
1	1	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	2	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	3	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	4	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	5	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	6	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	7	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	8	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	A	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	В	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	С	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	D	478/553~(86%)	467 (98%)	11 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	E	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	F	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	G	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	Н	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	I	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	J	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	K	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	L	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	M	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	N	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	О	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	Р	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	Q	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	R	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	S	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	Т	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	U	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	V	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	W	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	X	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	Y	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	Z	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	a	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	b	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	c	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	d	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	e	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	f	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	g	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	h	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	i	478/553~(86%)	467 (98%)	11 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	j	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	k	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	1	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	m	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	n	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	О	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	p	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	q	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	r	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	S	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	t	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	u	478/553 (86%)	467 (98%)	11 (2%)	0	100	100
1	V	478/553~(86%)	467 (98%)	11 (2%)	0	100	100
1	W	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	X	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	У	$478/553\ (86\%)$	467 (98%)	11 (2%)	0	100	100
1	Z	$478/553 \ (86\%)$	467 (98%)	11 (2%)	0	100	100
2	0	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	12	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	22	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	32	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	42	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	52	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	62	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	72	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	82	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	9	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	C2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	D2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	E2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	F2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	G2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	H2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	I2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	J2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	K2	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	L2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	M2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	N2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	O2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	P2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	Q2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	R2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	S2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	T2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	U2	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	V2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	W2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	X2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	Y2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	Z2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	a2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	b2	28/38 (74%)	25 (89%)	3 (11%)	0	100	100
2	c2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	d2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	e2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	f2	28/38 (74%)	26 (93%)	2 (7%)	0	100	100
2	g2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	h2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	i2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	j2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	k2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	12	28/38~(74%)	26 (93%)	2 (7%)	0	100	100
2	m2	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	n2	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	02	28/38~(74%)	26 (93%)	2 (7%)	0	100	100
2	p2	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	q2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	r2	28/38~(74%)	26 (93%)	2 (7%)	0	100	100
2	s2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	t2	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	u2	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	v2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	w2	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	x2	28/38~(74%)	27 (96%)	1 (4%)	0	100	100
2	y2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
2	z2	28/38 (74%)	27 (96%)	1 (4%)	0	100	100
All	All	30360/35460 (86%)	29620 (98%)	740 (2%)	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	ntiles
1	1	$420/478\ (88\%)$	417 (99%)	3 (1%)	84	93
1	2	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	3	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	4	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	5	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	6	420/478 (88%)	417 (99%)	3 (1%)	84	93



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	7	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	8	$420/478\ (88\%)$	417 (99%)	3 (1%)	84	93
1	A	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	В	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	С	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	D	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Е	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	F	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	G	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Н	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	I	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	J	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	K	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	L	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	M	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	N	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	О	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	P	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	Q	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	R	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	S	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Т	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	U	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	V	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	W	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	X	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Y	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	Z	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	a	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	b	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	c	420/478 (88%)	417 (99%)	3 (1%)	84	93



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	d	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	e	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	f	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	g	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	h	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	i	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	j	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	k	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	1	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	m	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	n	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	О	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	p	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	q	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	r	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	s	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	t	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	u	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	V	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	W	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	X	420/478 (88%)	417 (99%)	3 (1%)	84	93
1	У	420/478~(88%)	417 (99%)	3 (1%)	84	93
1	Z	420/478~(88%)	417 (99%)	3 (1%)	84	93
2	0	26/34~(76%)	26 (100%)	0	100	100
2	12	26/34~(76%)	26 (100%)	0	100	100
2	22	26/34 (76%)	26 (100%)	0	100	100
2	32	26/34 (76%)	26 (100%)	0	100	100
2	42	26/34~(76%)	26 (100%)	0	100	100
2	52	26/34 (76%)	26 (100%)	0	100	100
2	62	26/34 (76%)	26 (100%)	0	100	100
2	72	26/34 (76%)	26 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	82	26/34 (76%)	26 (100%)	0	100	100
2	9	26/34 (76%)	26 (100%)	0	100	100
2	C2	26/34~(76%)	26 (100%)	0	100	100
2	D2	26/34~(76%)	26 (100%)	0	100	100
2	E2	26/34~(76%)	26 (100%)	0	100	100
2	F2	26/34~(76%)	26 (100%)	0	100	100
2	G2	26/34~(76%)	26 (100%)	0	100	100
2	H2	26/34~(76%)	26 (100%)	0	100	100
2	I2	26/34~(76%)	26 (100%)	0	100	100
2	J2	26/34~(76%)	26 (100%)	0	100	100
2	K2	26/34 (76%)	26 (100%)	0	100	100
2	L2	26/34~(76%)	26 (100%)	0	100	100
2	M2	26/34~(76%)	26 (100%)	0	100	100
2	N2	26/34~(76%)	26 (100%)	0	100	100
2	O2	26/34~(76%)	26 (100%)	0	100	100
2	P2	26/34~(76%)	26 (100%)	0	100	100
2	Q2	26/34~(76%)	26 (100%)	0	100	100
2	R2	26/34~(76%)	26 (100%)	0	100	100
2	S2	26/34~(76%)	26 (100%)	0	100	100
2	T2	26/34~(76%)	26 (100%)	0	100	100
2	U2	26/34~(76%)	26 (100%)	0	100	100
2	V2	26/34 (76%)	26 (100%)	0	100	100
2	W2	26/34~(76%)	26 (100%)	0	100	100
2	X2	26/34~(76%)	26 (100%)	0	100	100
2	Y2	26/34~(76%)	26 (100%)	0	100	100
2	Z2	26/34 (76%)	26 (100%)	0	100	100
2	a2	26/34~(76%)	26 (100%)	0	100	100
2	b2	26/34 (76%)	26 (100%)	0	100	100
2	c2	26/34~(76%)	26 (100%)	0	100	100
2	d2	26/34~(76%)	26 (100%)	0	100	100
2	e2	26/34 (76%)	26 (100%)	0	100	100



 $Continued\ from\ previous\ page...$

Mol	Chain	Analysed	Rotameric	Outliers	Perce	$_{ m ntiles}$
2	f2	26/34~(76%)	26 (100%)	0	100	100
2	g2	26/34~(76%)	26 (100%)	0	100	100
2	h2	26/34 (76%)	26 (100%)	0	100	100
2	i2	26/34 (76%)	26 (100%)	0	100	100
2	j2	26/34 (76%)	26 (100%)	0	100	100
2	k2	26/34 (76%)	26 (100%)	0	100	100
2	12	26/34 (76%)	26 (100%)	0	100	100
2	m2	26/34 (76%)	26 (100%)	0	100	100
2	n2	26/34 (76%)	26 (100%)	0	100	100
2	02	26/34 (76%)	26 (100%)	0	100	100
2	p2	26/34 (76%)	26 (100%)	0	100	100
2	q2	26/34 (76%)	26 (100%)	0	100	100
2	r2	26/34 (76%)	26 (100%)	0	100	100
2	s2	26/34 (76%)	26 (100%)	0	100	100
2	t2	26/34 (76%)	26 (100%)	0	100	100
2	u2	26/34 (76%)	26 (100%)	0	100	100
2	v2	26/34 (76%)	26 (100%)	0	100	100
2	w2	26/34 (76%)	26 (100%)	0	100	100
2	x2	26/34 (76%)	26 (100%)	0	100	100
2	y2	26/34 (76%)	26 (100%)	0	100	100
2	z2	26/34 (76%)	26 (100%)	0	100	100
All	All	26760/30720 (87%)	26580 (99%)	180 (1%)	84	93

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	107	TRP
1	A	410	THR
1	В	96	LEU
1	В	107	TRP
1	В	410	THR
1	С	96	LEU
1	С	107	TRP
1	С	410	THR



Continued from previous page...

Conti	Continued from previous page					
Mol	Chain	Res	Type			
1	D	96	LEU			
1	D	107	TRP			
1	D	410	THR			
1	Е	96	LEU			
1	Е	107	TRP			
1	Е	410	THR			
1	F	96	LEU			
1	F	107	TRP			
1	F	410	THR			
1	G	96	LEU			
1	G	107	TRP			
1	G	410	THR			
1	Н	96	LEU			
1	Н	107	TRP			
1	Н	410	THR			
1	I	96	LEU			
1	I	107	TRP			
1	I	410	THR			
1	J	96	LEU			
1	J	107	TRP			
1	J	410	THR			
1	K	96	LEU			
1	K	107	TRP			
1	K	410	THR			
1	L	96	LEU			
1	L	107	TRP			
1	L	410	THR			
1	M	96	LEU			
1	M	107	TRP			
1	M	410	THR			
1	N	96	LEU			
1	N	107	TRP			
1	N	410	THR			
1	О	96	LEU			
1	О	107	TRP			
1	О	410	THR			
1	Р	96	LEU			
1	P	107	TRP			
1	Р	410	THR			
1	Q	96	LEU			
1	Q	107	TRP			
1	Q	410	THR			

 $\begin{array}{|c|c|c|c|c|c|}\hline Q & 410 & THR \\\hline Continued on next page... \\\hline \end{array}$



Continued from previous page...

Conti	Continued from previous page					
Mol	Chain	Res	Type			
1	R	96	LEU			
1	R	107	TRP			
1	R	410	THR			
1	S	96	LEU TRP			
1	S	107	TRP			
1	S T	410	THR			
1	Т	96	LEU			
1	Т	107	TRP THR			
1	T T	410				
1	U	96	LEU			
1	U	107	TRP			
1	U	410	THR			
1	V	96	LEU			
1	U V V	107	TRP			
1	V	410	THR			
1	W	96	LEU			
1	W	107	TRP			
1	W	410	THR			
1	X	96	LEU			
1	X	107	TRP			
1	X X Y Y	410	THR			
1	Y	96	LEU			
1	Y	107	TRP			
1	Y	410	THR			
1	Z	96	LEU TRP			
1	Z	107				
1	Z	410	THR			
1	a	96	LEU			
1	a	107	TRP			
1	a	410	THR			
1	b	96	LEU			
1	b	107	TRP			
1	b	410	THR			
1	c	96	LEU			
1	c	107	TRP			
1	С	410	THR			
1	d	96	LEU			
1	d	107	TRP			
1	d	410	THR			
1	е	96	LEU			
1	е	107	TRP			
1	е	410	THR			



Continued from previous page...

Conti	Continued from previous page					
Mol	Chain	Res	Type			
1	f	96	LEU			
1	f	107	TRP			
1	f	410	THR			
1	g	96	LEU			
1	g	107	TRP			
1	g	410	THR			
1	h	96	LEU			
1	h	107	TRP			
1	h	410	THR			
1	i	96	LEU			
1	i	107	TRP			
1	i	410	THR			
1	j	96	LEU			
1	j j j	107	TRP			
1	j	410	THR			
1	k	96	LEU			
1	k	107	TRP			
1	k	410	THR			
1	1	96	LEU			
1	1	107	TRP			
1	1	410	THR			
1	m	96	LEU			
1	m	107	TRP			
1	m	410	THR			
1	n	96	LEU			
1	n	107	TRP			
1	n	410	THR			
1	О	96	LEU			
1	О	107	TRP			
1	О	410	THR			
1	p	96	LEU			
1	p	107	TRP			
1	р	410	THR			
1	q	96	LEU			
1	q	107	TRP			
1	q	410	THR			
1	r	96	LEU			
1	r	107	TRP			
1	r	410	THR			
1	s	96	LEU			
1	s	107	TRP			
1	s	410	THR			



Continued from previous page

Conti	Continued from previous page					
Mol	Chain	Res	Type			
1	t	96	LEU			
1	t	107	TRP			
1	t	410	THR			
1	u	96	LEU			
1	u	107	TRP			
1	u	410	THR			
1	V	96	LEU			
1	V	107	TRP			
1	V	410	THR			
1	W	96	LEU			
1	W	107	TRP			
1	W	410	THR			
1	X	96	LEU			
1	X	107	TRP			
1	X	410	THR			
1	у	96	LEU			
1	У	107	TRP			
1	у	410	THR			
1	Z	96	LEU			
1	Z	107				
1	Z	410	TRP THR			
1	1	96	LEU			
1	1	107	TRP			
1	1	410	THR			
1	2	96	LEU			
1	2	107	TRP			
1	2	410	THR			
1	3	96	LEU			
1	3	107	TRP			
1	3	410	THR			
1	4	96	LEU			
1	4	107	TRP			
1	4	410	THR			
1	5	96	LEU			
1	5	107	TRP			
1	5	410	THR			
1	6	96	LEU			
1	6	107	TRP			
1	6	410	THR			
1	7	96	LEU			
1	7	107	TRP			
1	7	410	THR			
			ext page			
r						



Continued from previous page...

Mol	Chain	Res	Type
1	8	96	LEU
1	8	107	TRP
1	8	410	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (368) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A A A A	56	HIS
1	A	342	GLN
1	A	396	HIS
1	A	412	GLN
2 1	0	17	HIS
1	В	29	HIS
1	В	56	HIS
1	В	342	GLN
1	В	396	HIS
1	B C C C C D D	412	GLN
1	С	29	HIS
1	С	56	HIS
1	С	342	GLN HIS
1	С	396	HIS
1	С	412	GLN
1	D	29	HIS
1	D	56	HIS
1	D	342	GLN
1	D	396	HIS
1	D	412	GLN
1	Е	29	HIS
1	Е	56	HIS
1	Е	342	GLN
1	Е	396	HIS
1	Е	412	GLN
1	F	29	HIS
1	F	56	HIS
1	F	342	GLN
1	F	396	HIS
1	F	412	GLN
1	G G G	29	HIS
1	G	56	HIS
1	G	342	GLN
1	G	396	HIS



Continued from previous page...

			ous page
Mol	Chain	Res	Type
1	Н	29	HIS
1	Н	56	HIS
1	Н	342	GLN
1	Н	396	HIS
1	Н	412	GLN
1	I	29	HIS
1	I	56	HIS
1	I	342	GLN
1	I	396	HIS
1	I	412	GLN
1	J	29	HIS
1	J	56	HIS
1	J	342	GLN
1	J	396	HIS
1	J	412	GLN
1	K	29	HIS
1	K	56	HIS
1	K	164	GLN
1	K	342	GLN
1	K	396	HIS
1	K	412	GLN
1	L	29	HIS
1	L	56	HIS
1	L	342	GLN
1	L	396	HIS
1	L	412	GLN
1	M	29	HIS
1	M	56	HIS
1	M	342	GLN
1	M	396	HIS
1	M	412	GLN
1	N	29	HIS
1	N	56	HIS
1	N	342	GLN
1	N	396	HIS
1	N	412	GLN
1	О	29	HIS
1	О	56	HIS
1	О	342	GLN
1	О	396	HIS
1	О	412	GLN
1	Р	29	HIS



Continued from previous page...

	Continued from previous page					
Mol	Chain	Res	Type			
1	Р	56	HIS			
1	Р	342	GLN			
1	Р	396	HIS			
1	Р	412	GLN			
1	Q	29	HIS			
1	Q	56	HIS			
1	P P Q Q Q Q Q R	342	GLN			
1	Q	396	HIS			
1	Q	412	GLN			
1	R	29	HIS			
1	R	56	HIS			
1	R	164	GLN			
1	R	342	GLN			
1	R	396	HIS			
1	R	412	GLN			
1	S S	29	HIS			
1	S	56	HIS			
1	S	164	GLN			
1	S	342	GLN			
1	S	396	HIS			
1	S S S T T T T T T	29	HIS			
1	Т	56	HIS			
1	Т	164	GLN			
1	Т	342	GLN			
1	Т	396	HIS			
1	Т	412	GLN			
1	U	29	HIS			
1	U	56	HIS			
1	U	342	GLN			
1	U	396	HIS			
1	U	412	GLN			
1	V	29	HIS			
1	V	56	HIS			
1	V V V	164	GLN			
1	V	342	GLN			
1	V	396	HIS			
1	V	412	GLN			
1	W	29	HIS			
1	W	56	HIS			
1	W	342	GLN			
1	W	396	HIS			
1	W	412	GLN			



Continued from previous page...

Continued from previous page				
Mol	Chain	Res	Type	
1	X	29	HIS	
1	X	56	HIS	
1	X	342	GLN	
1	X	396	HIS	
1	X	412	GLN	
1	Y	29	HIS	
1	Y Y Y Y	56	HIS	
1	Y	342	GLN	
1	Y	396	HIS	
1	Y	412	GLN	
1	Y Z Z	29	HIS	
1	Z	56	HIS	
1	Z	164	GLN	
1	Z	342	GLN	
1	Z	396	HIS	
1	Z	412	GLN	
1	a	29	HIS	
1	a	56	HIS	
1	a	342	GLN	
1	a	396	HIS	
1	a	412	GLN	
1	b	29	HIS	
1	b	56	HIS	
1	b	342	GLN	
1	b	396	HIS	
1	b	412	GLN	
1	С	29	HIS	
1	С	56	HIS	
1	С	342	GLN	
1	С	396	HIS	
1	С	412	GLN	
1	d	29	HIS	
1	d	56	HIS	
1	d	342	GLN	
1	d	396	HIS	
1	d	412	GLN	
1	е	29	HIS	
1	е	56	HIS	
1	е	342	GLN	
1	е	396	HIS	
1	е	412	GLN	
1	f	29	HIS	



Continued from previous page...

	Continued from previous page				
Mol	Chain	Res	Type		
1	f	56	HIS		
1	f	342	GLN		
1	f	396	HIS		
1	f	412	GLN		
1	g	29	HIS		
1	g	56	HIS		
1	g	342	GLN		
1	g	396	HIS		
1	g	412	GLN		
1	h	29	HIS		
1	h	56	HIS		
1	h	342	GLN		
1	h	396	HIS		
1	h	412	GLN		
1	i	29	HIS		
1	i	56	HIS		
1	i	164	GLN		
1	i	342	GLN		
1	i	396	HIS		
1	i	412	GLN		
1	j	29	HIS		
1	j	56	HIS		
1	j	342	GLN		
1	j j	396	HIS		
1	j	412	GLN		
1	k	29	HIS		
1	k	56	HIS		
1	k	342	GLN		
1	k	396	HIS		
1	k	412	GLN		
1	1	29	HIS		
1	1	56	HIS		
1	1	342	GLN		
1	1	396	HIS		
1	1	412	GLN		
1	m	29	HIS		
1	m	56	HIS		
1	m	164	GLN		
1	m	342	GLN		
1	m	396	HIS		
1	m	412	GLN		
1	n	29	HIS		



Continued from previous page...

Mol	Chain	D	
	Chain	Res	Type
1	n	56	HIS
1	n	342	GLN
1	n	396	HIS
1	n	412	GLN
1	О	29	HIS
1	О	56	HIS
1	О	342	GLN
1	О	396	HIS
1	О	412	GLN
1	p	29	HIS
1	р	56	HIS
1	р	164	GLN
1	р	342	GLN
1	р	396	HIS
1	р	412	GLN
1	q	29	HIS
1	q	56	HIS
1	q	342	GLN
1	q	396	HIS
1	q	412	GLN
1	r	29	HIS
1	r	56	HIS
1	r	164	GLN
1	r	342	GLN
1	r	396	HIS
1	S	29	HIS
1	S	56	HIS
1	S	342	GLN
1	S	396	HIS
1	S	412	GLN
1	t	29	HIS
1	t	56	HIS
1	t	342	GLN
1	t	396	HIS
1	u	29	HIS
1	u	56	HIS
1	u	342	GLN
1	u	396	HIS
1	u	412	GLN
1	V	29	HIS
1	V	56	HIS
1	V	342	GLN



Continued from previous page...

Continued from previous page				
Mol	Chain	Res	Type	
1	V	396	HIS	
1	V	412	GLN	
1	V	449	GLN	
1	W	29	HIS	
1	W	56	HIS	
1	W	342	GLN	
1	W	396	HIS	
1	W	412	GLN	
1	X	29	HIS	
1	X	56	HIS	
1	X	342	GLN	
1	X	396	HIS	
1	X	412	GLN	
1	у	29	HIS	
1	у	56	HIS	
1	у	342	GLN	
1	у	396	HIS	
1	у	412	GLN	
1	Z	29	HIS	
1	Z	56	HIS	
1	Z	342	GLN	
1	Z	396	HIS	
1	Z	412	GLN	
1	1	29	HIS	
1	1	56	HIS	
1	1	342	GLN	
1	1	396	HIS	
1	1	412	GLN	
1	2	29	HIS	
1	2	56	HIS	
1	2	342	GLN	
1	2	396	HIS	
1		412	GLN	
1	3	29	HIS	
1	3	56	HIS	
1	3	342	GLN	
1	3	396	HIS	
1	3	412	GLN	
1	4	29	HIS	
1	4	56	HIS	
1	4	342	GLN	
1	4	396	HIS	



Continued from previous page...

	Continued from previous page				
Mol	Chain	Res	Type		
1	4	412	GLN		
1	5	29	HIS		
1	5	56	HIS		
1	5	164	GLN		
1	5	342	GLN		
1	5	396	HIS		
1	5	412	GLN		
1	6	29	HIS		
1	6	56	HIS		
1	6	342	GLN		
1	6	396	HIS		
1	6	412	GLN		
1	7	29	HIS		
1	7 7	56	HIS		
1	7	342	GLN		
1	7	396	HIS		
1	7	412	GLN		
1	8	29	HIS		
1	8	56	HIS		
1	8	164	GLN		
1	8	342	GLN		
1	8	396	HIS		
2	9	17	HIS		
2 2	C2	17	HIS		
2 2 2	D2	17	HIS		
2	E2	17	HIS		
2	F2	17	HIS		
2	G2	17	HIS		
2 2	H2	17	HIS		
2	I2	17	HIS		
2	J2	17	HIS		
2	K2	17	HIS		
2 2 2 2 2 2 2 2 2 2 2 2	L2	17 17	HIS		
2	M2	17	HIS		
2	N2	17	HIS		
2	O2	17	HIS		
2	P2	17	HIS		
2	Q2	17	HIS		
2	R2	17	HIS		
2	S2	17	HIS		
2	T2	17	HIS		
2	U2	17	HIS		



Mol	Chain	Res	Type HIS
2	V2	17	HIS
2	W2	17	HIS
2	X2	17	HIS
2	Y2	17 17	HIS HIS
2	Z2	17	HIS
2 2 2 2 2 2 2	W2 X2 Y2 Z2 a2	17	HIS
2	b2	17	HIS
2	c2	17	HIS
2	d2	17	HIS HIS
2	c2 d2 e2	17 17 17 17 17 17	HIS
2	f2	17	HIS HIS
2	g2	17	HIS
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	g2 h2 i2	17 17	HIS HIS
2	i2	17	HIS
2	j2	17	HIS
2	j2 k2	17 17 17 17 17 17	HIS
2	12	17	HIS HIS
2	m2	17	HIS
2	n2	17	HIS HIS
2	o2	17	HIS
2	p2	17	HIS
2	p2 q2 r2	17	HIS
2	r2	17	HIS
2	s2	17	HIS
2	t2	17	HIS
2	u2	17	HIS
2	v2	17	HIS
2 2 2 2	v2 w2	17 17	HIS
2	x2	17	HIS
2	y2	17	HIS
2	z2	17	HIS
2	12	17	HIS
2	22	17	HIS
2	32	17	HIS
2 2 2 2 2 2 2 2	42	17	HIS
2	52	17	HIS
2	62	17	HIS
2	72	17	HIS
2	82	17	HIS



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.



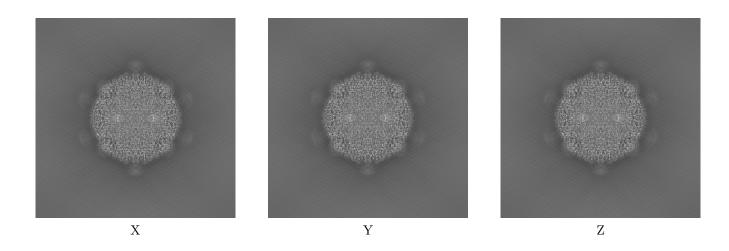
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-45583. These allow visual inspection of the internal detail of the map and identification of artifacts.

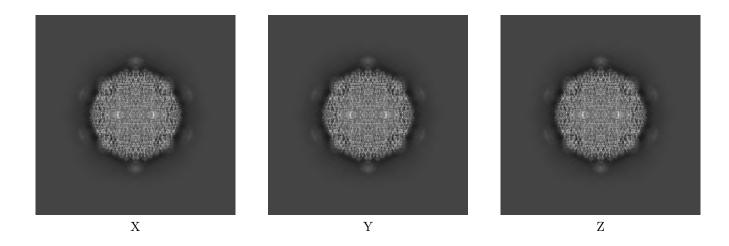
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

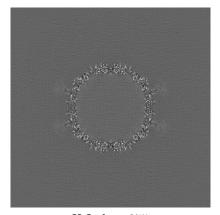


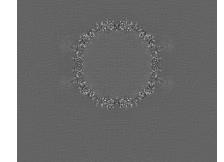
The images above show the map projected in three orthogonal directions.

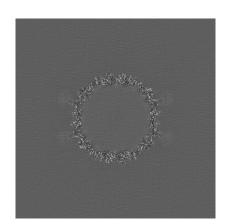


6.2 Central slices (i)

6.2.1 Primary map





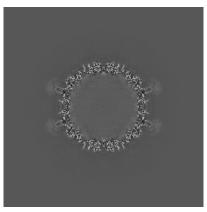


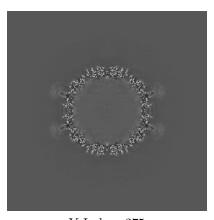
X Index: 275

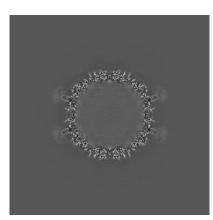
Y Index: 275

Z Index: 275

6.2.2 Raw map







X Index: 275

Y Index: 275

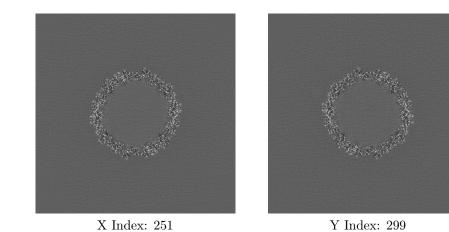
Z Index: 275

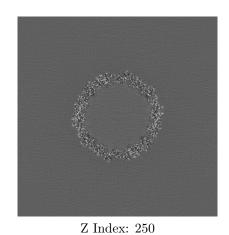
The images above show central slices of the map in three orthogonal directions.



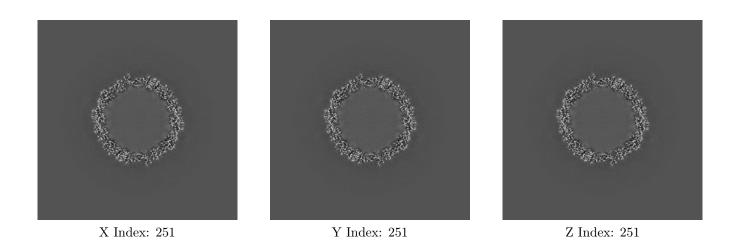
6.3 Largest variance slices (i)

6.3.1 Primary map





6.3.2 Raw map

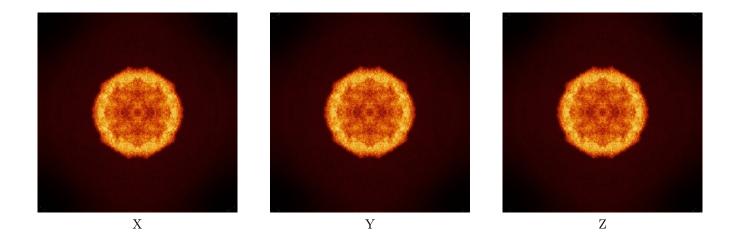


The images above show the largest variance slices of the map in three orthogonal directions.

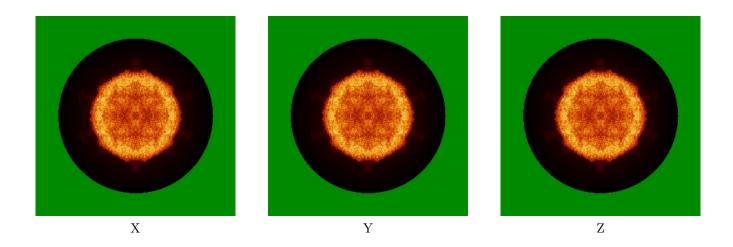


6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map

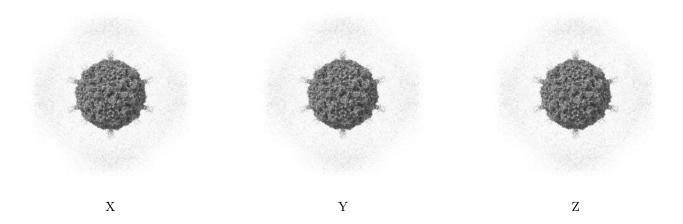


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



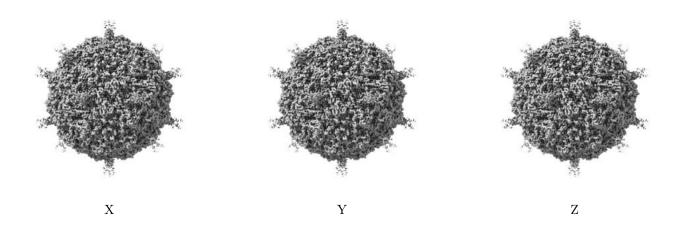
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. 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)

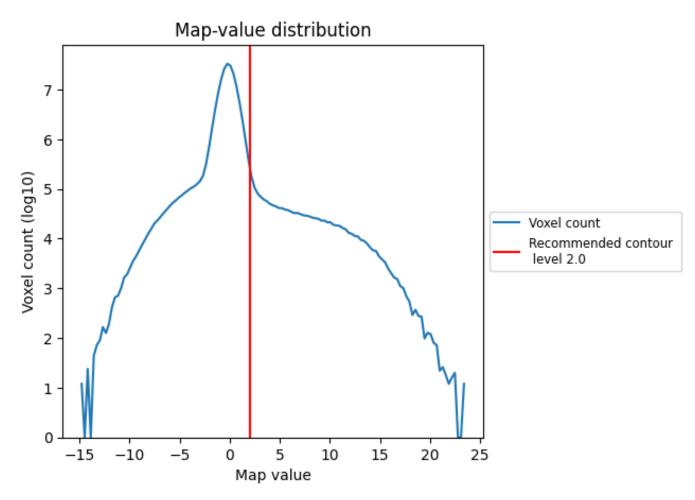
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

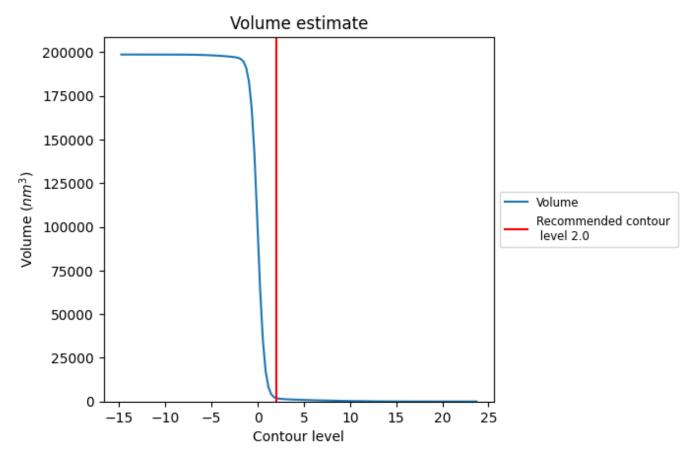
7.1 Map-value distribution (i)



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)

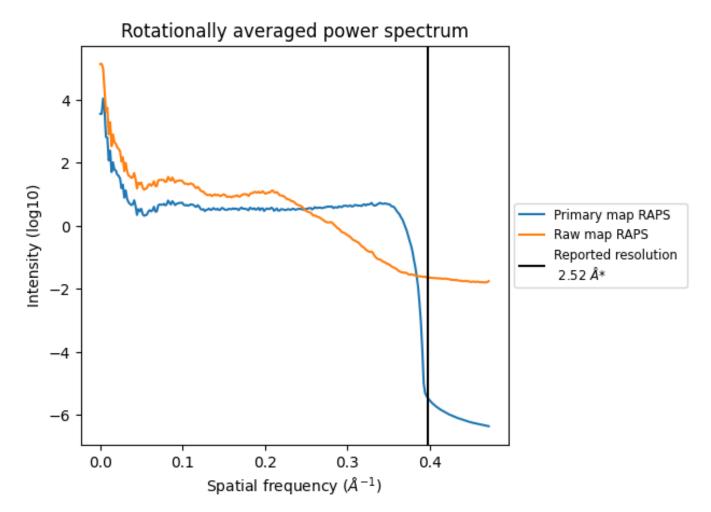


The volume at the recommended contour level is $1990~\mathrm{nm^3}$; this corresponds to an approximate mass of $1798~\mathrm{kDa}$.

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)



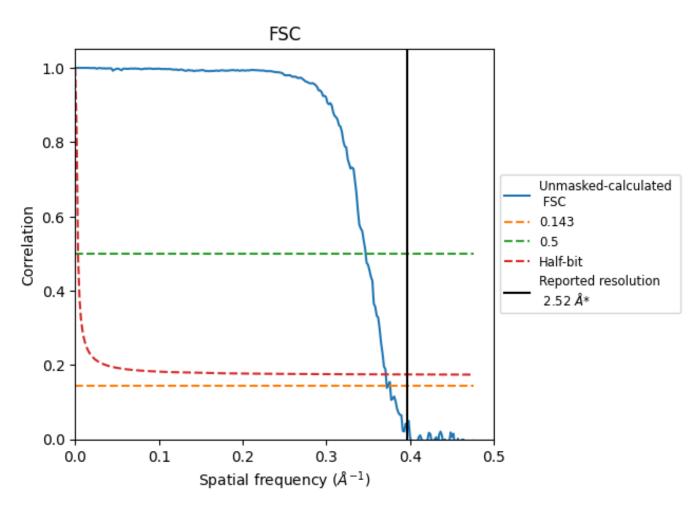
^{*}Reported resolution corresponds to spatial frequency of 0.397 $\rm \mathring{A}^{-1}$



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 0.397 $\rm \mathring{A}^{-1}$



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	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.69	2.88	2.70

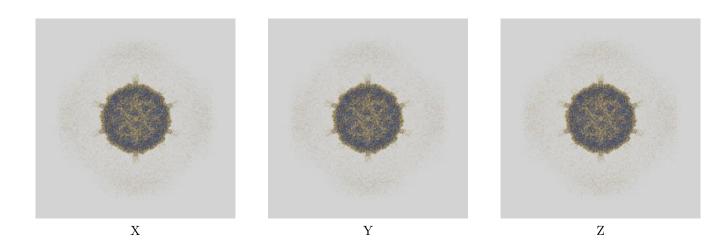
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-45583 and PDB model 9CGM. Per-residue inclusion information can be found in section 3 on page 14.

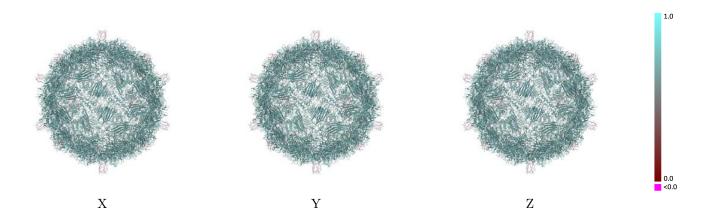
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

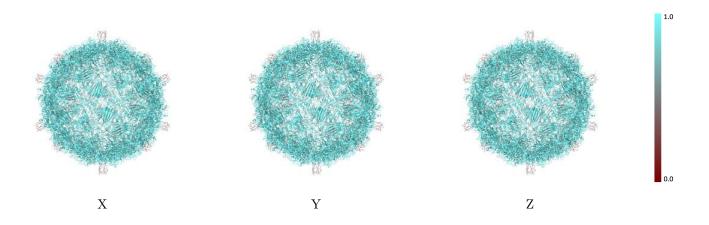


9.2 Q-score mapped to coordinate model (i)



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

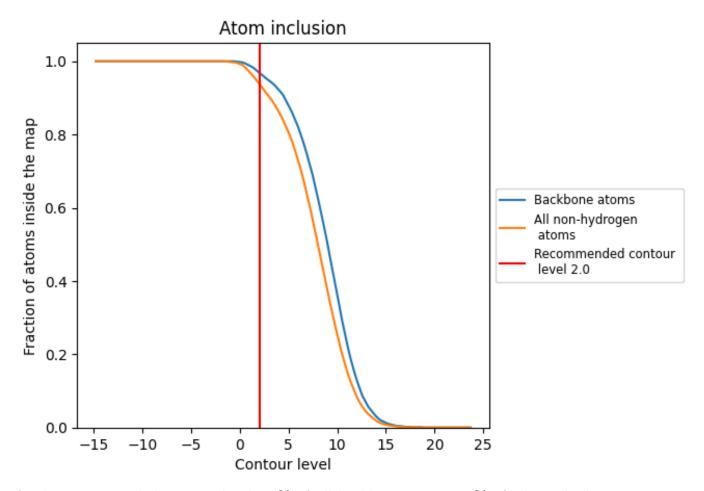
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.0).



9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.6470
0	0.8160	0.5870
1	0.9460	0.6510
12	0.8120	0.5890
2	0.9460	0.6530
22	0.8120	0.5880
3	0.9450	0.6510
32	0.8030	0.5900
4	0.9470	0.6510
42	0.8070	0.5860
5	0.9480	0.6510
52	0.8070	0.5880
6	0.9470	0.6510
62	0.8070	0.5920
7	0.9470	0.6510
72	0.8070	0.5900
8	0.9490	0.6520
82	0.7990	0.5820
9	0.8120	0.5850
A	0.9450	0.6510
В	0.9460	0.6510
С	0.9470	0.6510
C2	0.8070	0.5850
D	0.9470	0.6520
D2	0.8070	0.5880
E	0.9490	0.6510
E2	0.7990	0.5840
F	0.9450	0.6510
F2	0.8030	0.5860
G	0.9490	0.6510
G2	0.7990	0.5800
Н	0.9470	0.6510
H2	0.8070	0.5840
I	0.9470	0.6500
I2	0.8070	0.5810





Chain	Atom inclusion	Q-score
J	0.9460	0.6510
J2	0.8120	0.5850
K	0.9470	0.6520
K2	0.8070	0.5840
L	0.9460	0.6520
L2	0.8120	0.5840
M	0.9490	0.6520
M2	0.7990	0.5760
N	0.9470	0.6510
N2	0.8070	0.5870
О	0.9490	0.6520
O2	0.7990	0.5820
Р	0.9470	0.6510
P2	0.8070	0.5890
Q	0.9470	0.6520
Q2	0.8070	0.5830
R	0.9460	0.6520
R2	0.8120	0.5890
S	0.9460	0.6510
S2	0.8120	0.5860
Т	0.9470	0.6520
T2	0.8070	0.5870
U	0.9460	0.6520
U2	0.8120	0.5840
V	0.9470	0.6510
V2	0.8070	0.5880
W	0.9470	0.6510
W2	0.8070	0.5880
X	0.9490	0.6520
X2	0.7990	0.5830
Y	0.9470	0.6510
Y2	0.8070	0.5900
Z	0.9490	0.6520
Z2	0.7990	0.5820
a	0.9450	0.6520
a2	0.8030	0.5900
b	0.9450	0.6520
b2	0.8030	0.5910
С	0.9450	0.6510
c2	0.8030	0.5900
d	0.9450	0.6520
d2	0.8030	0.5860



 $Continued\ from\ previous\ page...$

Chain	Atom inclusion	Q-score
e	0.9450	0.6520
e2	0.8030	0.5900
f	0.9450	0.6520
f2	0.8030	0.5920
g	0.9470	0.6510
g2	0.8070	0.5820
h	0.9490	0.6510
h2	0.7950	0.5770
i	0.9470	0.6520
i2	0.8070	0.5870
j	0.9480	0.6510
j2	0.8070	0.5880
k	0.9470	0.6510
k2	0.8070	0.5880
1	0.9490	0.6520
12	0.7990	0.5820
m	0.9470	0.6520
m2	0.8070	0.5860
n	0.9450	0.6530
n2	0.8030	0.5890
О	0.9490	0.6510
02	0.7990	0.5800
p	0.9470	0.6520
p2	0.8070	0.5860
q	0.9460	0.6510
q2	0.8120	0.5860
r	0.9460	0.6500
r2	0.8120	0.5880
S	0.9460	0.6510
s2	0.8120	0.5840
t	0.9490	0.6520
t2	0.7990	0.5830
u	0.9470	0.6510
u2	0.8070	0.5840
V	0.9450	0.6510
v2	0.8070	0.5860
W	0.9490	0.6510
w2	0.7990	0.5810
X	0.9470	0.6500
x2	0.8070	0.5840
У	0.9450	0.6500
y2	0.8070	0.5890



Chain	Atom inclusion	Q-score
Z	0.9460	0.6520
z2	0.8120	0.5830

