Full wwPDB EM Validation Report (i)

May 1, 2024 – 12:44 am BST

PDB ID	:	4CTF
EMDB ID	:	EMD-2389
Title	:	The limits of structural plasticity in a picornavirus capsid revealed by a massively expanded equine rhinitis A virus particle
Authors	:	Bakker, S.E.; Groppelli, E.; Pearson, A.R.; Stockley, P.G.; Rowlands, D.J.; Ranson, N.A.
Deposited on	:	2014-03-13
Resolution	:	17.00 Å(reported)
Based on initial model	:	2WFF

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

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 17.00 Å.

There are no overall percentile quality scores available for this entry.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 321060 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A0	246	1929	1240	329	352	8	0	0
1	A1	246	1929	1240	329	352	8	0	0
1	A2	246	1929	1240	329	352	8	0	0
1	A3	246	1929	1240	329	352	8	0	0
1	A4	246	1929	1240	329	352	8	0	0
1	A5	246	1929	1240	329	352	8	0	0
1	A6	246	1929	1240	329	352	8	0	0
1	A7	246	1929	1240	329	352	8	0	0
1	A8	246	1929	1240	329	352	8	0	0
1	A9	246	1929	1240	329	352	8	0	0
1	AA	246	1929	1240	329	352	8	0	0
1	AB	246	1929	1240	329	352	8	0	0
1	AC	246	1929	1240	329	352	8	0	0
1	AD	246	1929	1240	329	352	8	0	0
1	AE	246	1929	1240	329	352	8	0	0
1	AF	246	1929	1240	329	352	8	0	0
1	AG	246	1929	1240	329	352	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AH	246	1929	1240	329	352	8	0	0
1	AI	246	1929	1240	329	352	8	0	0
1	AJ	246	1929	1240	329	352	8	0	0
1	AK	246	1929	1240	329	352	8	0	0
1	AL	246	1929	1240	329	352	8	0	0
1	AM	246	1929	1240	329	352	8	0	0
1	AN	246	1929	1240	329	352	8	0	0
1	AO	246	1929	1240	329	352	8	0	0
1	AP	246	1929	1240	329	352	8	0	0
1	AQ	246	1929	1240	329	352	8	0	0
1	AR	246	1929	1240	329	352	8	0	0
1	AS	246	1929	1240	329	352	8	0	0
1	AT	246	1929	1240	329	352	8	0	0
1	AU	246	1929	1240	329	352	8	0	0
1	AV	246	1929	1240	329	352	8	0	0
1	AW	246	1929	1240	329	352	8	0	0
1	AX	246	1929	1240	329	352	8	0	0
1	AY	246	1929	1240	329	352	8	0	0
1	AZ	246	1929	1240	329	352	8	0	0
1	Aa	246	1929	1240	329	352	8	0	0
1	Ab	246	1929	1240	329	352	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Ac	246	1929	1240	329	352	8	0	0
1	Ad	246	1929	1240	329	352	8	0	0
1	Ae	246	1929	1240	329	352	8	0	0
1	Af	246	1929	1240	329	352	8	0	0
1	Ag	246	1929	1240	329	352	8	0	0
1	Ah	246	1929	1240	329	352	8	0	0
1	Ai	246	1929	1240	329	352	8	0	0
1	Aj	246	1929	1240	329	352	8	0	0
1	Ak	246	1929	1240	329	352	8	0	0
1	Al	246	1929	1240	329	352	8	0	0
1	Am	246	1929	1240	329	352	8	0	0
1	An	246	1929	1240	329	352	8	0	0
1	Ao	246	1929	1240	329	352	8	0	0
1	BA	246	1929	1240	329	352	8	0	0
1	BB	246	1929	1240	329	352	8	0	0
1	BC	246	1929	1240	329	352	8	0	0
1	BD	246	1929	1240	329	352	8	0	0
1	BE	246	1929	1240	329	352	8	0	0
1	BF	246	1929	1240	329	352	8	0	0
1	BG	246	1929	1240	329	352	8	0	0
1	BH	246	1929	1240	329	352	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BI	246	1929	1240	329	352	8	0	0

- Molecule 2 is a protein called EQUINE RHINITIS A VIRUS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C0	198	1537	986	261	286	4	0	0
2	C1	198	1537	986	261	286	4	0	0
2	C2	198	1537	986	261	286	4	0	0
2	C3	198	1537	986	261	286	4	0	0
2	C4	198	1537	986	261	286	4	0	0
2	C5	198	1537	986	261	286	4	0	0
2	C6	198	1537	986	261	286	4	0	0
2	C7	198	1537	986	261	286	4	0	0
2	C8	198	1537	986	261	286	4	0	0
2	C9	198	1537	986	261	286	4	0	0
2	CA	198	1537	986	261	286	4	0	0
2	CB	198	1537	986	261	286	4	0	0
2	CC	198	1537	986	261	286	4	0	0
2	CD	198	1537	986	261	286	4	0	0
2	CE	198	1537	986	261	286	4	0	0
2	CF	198	1537	986	261	286	4	0	0
2	CG	198	1537	986	261	286	4	0	0
2	CH	198	1537	986	261	286	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CI	198	1537	986	261	286	4	0	0
2	CJ	198	1537	986	261	286	4	0	0
2	CK	198	1537	986	261	286	4	0	0
2	CL	198	1537	986	261	286	4	0	0
2	CM	198	1537	986	261	286	4	0	0
2	CN	198	1537	986	261	286	4	0	0
2	CO	198	1537	986	261	286	4	0	0
2	CP	198	1537	986	261	286	4	0	0
2	CQ	198	1537	986	261	286	4	0	0
2	CR	198	1537	986	261	286	4	0	0
2	CS	198	1537	986	261	286	4	0	0
2	CT	198	1537	986	261	286	4	0	0
2	CU	198	1537	986	261	286	4	0	0
2	CV	198	1537	986	261	286	4	0	0
2	CW	198	1537	986	261	286	4	0	0
2	CX	198	1537	986	261	286	4	0	0
2	CY	198	1537	986	261	286	4	0	0
2	CZ	198	1537	986	261	286	4	0	0
2	Ca	198	1537	986	261	286	4	0	0
2	Cb	198	1537	986	261	286	4	0	0
2	Cc	198	1537	986	261	286	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Cd	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Ce	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cf	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cg	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Ch	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Ci	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cj	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Ck	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cl	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cm	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cn	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Co	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cp	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cq	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cr	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cs	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Ct	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cu	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cv	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cw	198	1537	986	261	286	4	0	0
			Total	C	N	O	S		
2	Cx	198	1537	986	261	286	4	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	85	SER	GLY	conflict	UNP Q91B42
C1	85	SER	GLY	conflict	UNP Q91B42
C2	85	SER	GLY	conflict	UNP Q91B42
C3	85	SER	GLY	conflict	UNP Q91B42
C4	85	SER	GLY	conflict	UNP Q91B42
C5	85	SER	GLY	conflict	UNP Q91B42
C6	85	SER	GLY	conflict	UNP Q91B42
C7	85	SER	GLY	conflict	UNP Q91B42
C8	85	SER	GLY	conflict	UNP Q91B42
C9	85	SER	GLY	conflict	UNP Q91B42
CA	85	SER	GLY	conflict	UNP Q91B42
CB	85	SER	GLY	conflict	UNP Q91B42
CC	85	SER	GLY	conflict	UNP Q91B42
CD	85	SER	GLY	conflict	UNP Q91B42
CE	85	SER	GLY	conflict	UNP Q91B42
CF	85	SER	GLY	conflict	UNP Q91B42
CG	85	SER	GLY	conflict	UNP Q91B42
CH	85	SER	GLY	conflict	UNP Q91B42
CI	85	SER	GLY	conflict	UNP Q91B42
CJ	85	SER	GLY	conflict	UNP Q91B42
CK	85	SER	GLY	conflict	UNP Q91B42
CL	85	SER	GLY	conflict	UNP Q91B42
CM	85	SER	GLY	conflict	UNP Q91B42
CN	85	SER	GLY	conflict	UNP Q91B42
CO	85	SER	GLY	conflict	UNP Q91B42
CP	85	SER	GLY	conflict	UNP Q91B42
CQ	85	SER	GLY	conflict	UNP Q91B42
CR	85	SER	GLY	conflict	UNP Q91B42
CS	85	SER	GLY	conflict	UNP Q91B42
CT	85	SER	GLY	conflict	UNP Q91B42
CU	85	SER	GLY	conflict	UNP Q91B42
CV	85	SER	GLY	conflict	UNP Q91B42
CW	85	SER	GLY	conflict	UNP Q91B42
CX	85	SER	GLY	conflict	UNP Q91B42
CY	85	SER	GLY	conflict	UNP Q91B42
CZ	85	SER	GLY	conflict	UNP Q91B42
Ca	85	SER	GLY	conflict	UNP Q91B42
Cb	85	SER	GLY	conflict	UNP Q91B42
Cc	85	SER	GLY	conflict	UNP Q91B42
Cd	85	SER	GLY	conflict	UNP Q91B42
Ce	85	SER	GLY	conflict	UNP Q91B42
Cf	85	SER	GLY	conflict	UNP Q91B42

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Chain	Residue	Modelled	Actual	Comment	Reference
Cg	85	SER	GLY	conflict	UNP Q91B42
Ch	85	SER	GLY	conflict	UNP Q91B42
Ci	85	SER	GLY	conflict	UNP Q91B42
Cj	85	SER	GLY	conflict	UNP Q91B42
Ck	85	SER	GLY	conflict	UNP Q91B42
Cl	85	SER	GLY	conflict	UNP Q91B42
Cm	85	SER	GLY	conflict	UNP Q91B42
Cn	85	SER	GLY	conflict	UNP Q91B42
Co	85	SER	GLY	conflict	UNP Q91B42
Cp	85	SER	GLY	conflict	UNP Q91B42
Cq	85	SER	GLY	conflict	UNP Q91B42
Cr	85	SER	GLY	conflict	UNP Q91B42
Cs	85	SER	GLY	conflict	UNP Q91B42
Ct	85	SER	GLY	conflict	UNP Q91B42
Cu	85	SER	GLY	conflict	UNP Q91B42
Cv	85	SER	GLY	conflict	UNP Q91B42
Cw	85	SER	GLY	conflict	UNP Q91B42
Cx	85	SER	GLY	conflict	UNP Q91B42

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D0	226	1719	1107	280	326	6	0	0
3	D1	226	1719	1107	280	326	6	0	0
3	D2	226	1719	1107	280	326	6	0	0
3	D3	226	1719	1107	280	326	6	0	0
3	D4	226	1719	1107	280	326	6	0	0
3	D5	226	1719	1107	280	326	6	0	0
3	D6	226	1719	1107	280	326	6	0	0
3	D7	226	1719	1107	280	326	6	0	0
3	D8	226	1719	1107	280	326	6	0	0
3	D9	226	1719	1107	280	326	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	DA	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DB	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DC	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DD	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DE	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DF	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DG	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DH	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DI	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DJ	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DK	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DL	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DM	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DN	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DO	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DP	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DQ	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DR	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DS	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DT	226	1719	1107	280	326	6	0	0
			Total	C	N	O	S		
3	DU	226	1719	1107	280	326	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	DV	226	1719	1107	280	326	6	0	0
3	DW	226	1719	1107	280	326	6	0	0
3	DX	226	1719	1107	280	326	6	0	0
3	DY	226	1719	1107	280	326	6	0	0
3	DZ	226	1719	1107	280	326	6	0	0
3	Da	226	1719	1107	280	326	6	0	0
3	Db	226	1719	1107	280	326	6	0	0
3	Dc	226	1719	1107	280	326	6	0	0
3	Dd	226	1719	1107	280	326	6	0	0
3	De	226	1719	1107	280	326	6	0	0
3	Df	226	1719	1107	280	326	6	0	0
3	Dg	226	1719	1107	280	326	6	0	0
3	Dh	226	1719	1107	280	326	6	0	0
3	Di	226	1719	1107	280	326	6	0	0
3	Dj	226	1719	1107	280	326	6	0	0
3	Dk	226	1719	1107	280	326	6	0	0
3	Dl	226	1719	1107	280	326	6	0	0
3	Dm	226	1719	1107	280	326	6	0	0
3	Dn	226	1719	1107	280	326	6	0	0
3	Do	226	1719	1107	280	326	6	0	0
3	Dp	226	1719	1107	280	326	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Dq	226	1719	1107	280	326	6	0	0
3	Dr	226	1719	1107	280	326	6	0	0
3	Ds	226	1719	1107	280	326	6	0	0
3	EA	226	1719	1107	280	326	6	0	0
3	EB	226	1719	1107	280	326	6	0	0
3	EC	226	1719	1107	280	326	6	0	0
3	ED	226	1719	1107	280	326	6	0	0
3	EE	226	1719	1107	280	326	6	0	0

- Molecule 4 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F0	22	166	101	29	35	1	0	1
4	F1	22	166	101	29	35	1	0	1
4	F2	22	166	101	29	35	1	0	1
4	F3	22	166	101	29	35	1	0	1
4	F4	22	166	101	29	35	1	0	1
4	F5	22	166	101	29	35	1	0	1
4	F6	22	166	101	29	35	1	0	1
4	F7	22	166	101	29	35	1	0	1
4	F8	22	166	101	29	35	1	0	1
4	F9	22	166	101	29	35	1	0	1
4	FA	22	166	101	29	35	1	0	1

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	FB	22	166	101	29	35	1	0	1
4	FC	22	166	101	29	35	1	0	1
4	FD	22	166	101	29	35	1	0	1
4	FE	22	166	101	29	35	1	0	1
4	FF	22	166	101	29	35	1	0	1
4	FG	22	166	101	29	35	1	0	1
4	FH	22	166	101	29	35	1	0	1
4	FI	22	166	101	29	35	1	0	1
4	FJ	22	166	101	29	35	1	0	1
4	FK	22	166	101	29	35	1	0	1
4	FL	22	166	101	29	35	1	0	1
4	FM	22	166	101	29	35	1	0	1
4	FN	22	166	101	29	35	1	0	1
4	FO	22	166	101	29	35	1	0	1
4	FP	22	166	101	29	35	1	0	1
4	FQ	22	166	101	29	35	1	0	1
4	FR	22	166	101	29	35	1	0	1
4	FS	22	166	101	29	35	1	0	1
4	FT	22	166	101	29	35	1	0	1
4	FU	22	166	101	29	35	1	0	1
4	FV	22	166	101	29	35	1	0	1

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	FW	22	166	101	29	35	1	0	1
4	FX	22	166	101	29	35	1	0	1
4	FY	22	166	101	29	35	1	0	1
4	FZ	22	166	101	29	35	1	0	1
4	Fa	22	166	101	29	35	1	0	1
4	Fb	22	166	101	29	35	1	0	1
4	Fc	22	166	101	29	35	1	0	1
4	Fd	22	166	101	29	35	1	0	1
4	Fe	22	166	101	29	35	1	0	1
4	Ff	22	166	101	29	35	1	0	1
4	Fg	22	166	101	29	35	1	0	1
4	Fh	22	166	101	29	35	1	0	1
4	Fi	22	166	101	29	35	1	0	1
4	Fj	22	166	101	29	35	1	0	1
4	Fk	22	166	101	29	35	1	0	1
4	Fl	22	166	101	29	35	1	0	1
4	Fm	22	166	101	29	35	1	0	1
4	Fn	22	166	101	29	35	1	0	1
4	Fo	22	166	101	29	35	1	0	1
4	Fp	22	166	101	29	35	1	0	1
4	Fq	22	166	101	29	35	1	0	1

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Fr	22	166	101	29	35	1	0	1
			Total	C	N	O	S		
4	Fs	22	166	101	29	35	1	0	1
			Total	C	N	O	S		
4	Ft	22	166	101	29	35	1	0	1
			Total	C	N	O	S		
4	Fu	22	166	101	29	35	1	0	1
			Total	C	N	O	S		
4	Fv	22	166	101	29	35	1	0	1
			Total	C	N	O	S		
4	Fw	22	166	101	29	35	1	0	1
			Total	C	N	O	S		
4	Fx	22	166	101	29	35	1	0	1

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	260	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING, EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	15	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	87209	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2389. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

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

6 Map analysis (i)

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

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit (i)

This section was not generated.