



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 05:33 PM JST

PDB ID : 7FDJ
EMDB ID : EMD-31545
Title : Engineered Hepatitis B virus core antigen with short linker T=4
Authors : Jeong, H.; Heo, Y.; Yoo, Y.; Ryu, B.; Yun, J.; Cho, H.; Lee, W.
Deposited on : 2021-07-16
Resolution : 4.40 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
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) : 2.31.3

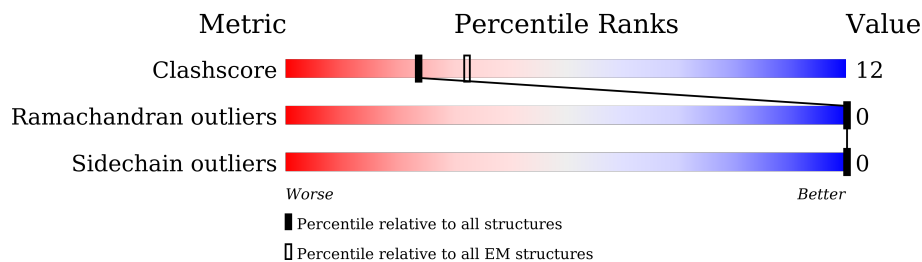
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	
1	B	318	
1	C	318	
1	D	318	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4416 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,Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	137	1104	722	179	198	5	0	0
1	B	137	1104	722	179	198	5	0	0
1	D	137	1104	722	179	198	5	0	0
1	C	137	1104	722	179	198	5	0	0

There are 344 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P69706
A	2	HIS	-	expression tag	UNP P69706
A	3	HIS	-	expression tag	UNP P69706
A	4	HIS	-	expression tag	UNP P69706
A	5	HIS	-	expression tag	UNP P69706
A	6	HIS	-	expression tag	UNP P69706
A	7	HIS	-	expression tag	UNP P69706
A	8	MET	-	expression tag	UNP P69706
A	9	ALA	-	expression tag	UNP P69706
A	10	SER	-	expression tag	UNP P69706
A	11	SER	-	expression tag	UNP P69706
A	12	LEU	-	expression tag	UNP P69706
A	13	ARG	-	expression tag	UNP P69706
A	14	GLN	-	expression tag	UNP P69706
A	15	ILE	-	expression tag	UNP P69706
A	16	LEU	-	expression tag	UNP P69706
A	17	ASP	-	expression tag	UNP P69706
A	18	SER	-	expression tag	UNP P69706
A	19	GLN	-	expression tag	UNP P69706
A	20	LYS	-	expression tag	UNP P69706
A	21	MET	-	expression tag	UNP P69706
A	22	GLU	-	expression tag	UNP P69706

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	TRP	-	expression tag	UNP P69706
A	24	ARG	-	expression tag	UNP P69706
A	25	SER	-	expression tag	UNP P69706
A	26	ASN	-	expression tag	UNP P69706
A	27	ALA	-	expression tag	UNP P69706
A	28	GLY	-	expression tag	UNP P69706
A	29	GLY	-	expression tag	UNP P69706
A	30	SER	-	expression tag	UNP P69706
A	31	GLY	-	expression tag	UNP P69706
A	32	GLY	-	expression tag	UNP P69706
A	33	GLY	-	expression tag	UNP P69706
A	34	SER	-	expression tag	UNP P69706
A	35	GLY	-	expression tag	UNP P69706
A	36	GLY	-	expression tag	UNP P69706
A	37	GLY	-	expression tag	UNP P69706
A	38	THR	-	expression tag	UNP P69706
A	39	GLY	-	expression tag	UNP P69706
A	40	GLY	-	expression tag	UNP P69706
A	41	GLY	-	expression tag	UNP P69706
A	42	GLY	-	expression tag	UNP P69706
A	43	GLY	-	expression tag	UNP P69706
A	44	GLY	-	expression tag	UNP P69706
A	45	TYR	-	expression tag	UNP P69706
A	46	TYR	-	expression tag	UNP P69706
A	47	TYR	-	expression tag	UNP P69706
A	48	TYR	-	expression tag	UNP P69706
A	49	TYR	-	expression tag	UNP P69706
A	50	TYR	-	expression tag	UNP P69706
A	128	LEU	-	linker	UNP P69706
A	129	GLU	-	linker	UNP P69706
A	130	VAL	ALA	engineered mutation	UNP P38507
A	138	MET	GLN	engineered mutation	UNP P38507
A	139	TRP	GLN	engineered mutation	UNP P38507
A	140	ALA	ASN	engineered mutation	UNP P38507
A	142	TRP	PHE	engineered mutation	UNP P38507
A	143	GLU	TYR	engineered mutation	UNP P38507
A	146	ARG	LEU	engineered mutation	UNP P38507
A	147	ASN	HIS	engineered mutation	UNP P38507
A	153	GLY	GLU	engineered mutation	UNP P38507
A	154	TRP	GLU	engineered mutation	UNP P38507
A	156	MET	ARG	engineered mutation	UNP P38507
A	157	THR	ASN	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ALA	GLY	engineered mutation	UNP P38507
A	161	ALA	GLN	engineered mutation	UNP P38507
A	164	VAL	LYS	engineered mutation	UNP P38507
A	188	GLU	-	linker	UNP P38507
A	189	PHE	-	linker	UNP P38507
A	190	VAL	ALA	engineered mutation	UNP P38507
A	198	MET	GLN	engineered mutation	UNP P38507
A	199	TRP	GLN	engineered mutation	UNP P38507
A	200	ALA	ASN	engineered mutation	UNP P38507
A	202	TRP	PHE	engineered mutation	UNP P38507
A	203	GLU	TYR	engineered mutation	UNP P38507
A	206	ARG	LEU	engineered mutation	UNP P38507
A	207	ASN	HIS	engineered mutation	UNP P38507
A	213	GLY	GLU	engineered mutation	UNP P38507
A	214	TRP	GLU	engineered mutation	UNP P38507
A	216	MET	ARG	engineered mutation	UNP P38507
A	217	THR	ASN	engineered mutation	UNP P38507
A	218	ALA	GLY	engineered mutation	UNP P38507
A	221	ALA	GLN	engineered mutation	UNP P38507
A	224	VAL	LYS	engineered mutation	UNP P38507
A	248	GLY	-	linker	UNP P38507
A	249	SER	-	linker	UNP P38507
B	1	MET	-	initiating methionine	UNP P69706
B	2	HIS	-	expression tag	UNP P69706
B	3	HIS	-	expression tag	UNP P69706
B	4	HIS	-	expression tag	UNP P69706
B	5	HIS	-	expression tag	UNP P69706
B	6	HIS	-	expression tag	UNP P69706
B	7	HIS	-	expression tag	UNP P69706
B	8	MET	-	expression tag	UNP P69706
B	9	ALA	-	expression tag	UNP P69706
B	10	SER	-	expression tag	UNP P69706
B	11	SER	-	expression tag	UNP P69706
B	12	LEU	-	expression tag	UNP P69706
B	13	ARG	-	expression tag	UNP P69706
B	14	GLN	-	expression tag	UNP P69706
B	15	ILE	-	expression tag	UNP P69706
B	16	LEU	-	expression tag	UNP P69706
B	17	ASP	-	expression tag	UNP P69706
B	18	SER	-	expression tag	UNP P69706
B	19	GLN	-	expression tag	UNP P69706
B	20	LYS	-	expression tag	UNP P69706

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	MET	-	expression tag	UNP P69706
B	22	GLU	-	expression tag	UNP P69706
B	23	TRP	-	expression tag	UNP P69706
B	24	ARG	-	expression tag	UNP P69706
B	25	SER	-	expression tag	UNP P69706
B	26	ASN	-	expression tag	UNP P69706
B	27	ALA	-	expression tag	UNP P69706
B	28	GLY	-	expression tag	UNP P69706
B	29	GLY	-	expression tag	UNP P69706
B	30	SER	-	expression tag	UNP P69706
B	31	GLY	-	expression tag	UNP P69706
B	32	GLY	-	expression tag	UNP P69706
B	33	GLY	-	expression tag	UNP P69706
B	34	SER	-	expression tag	UNP P69706
B	35	GLY	-	expression tag	UNP P69706
B	36	GLY	-	expression tag	UNP P69706
B	37	GLY	-	expression tag	UNP P69706
B	38	THR	-	expression tag	UNP P69706
B	39	GLY	-	expression tag	UNP P69706
B	40	GLY	-	expression tag	UNP P69706
B	41	GLY	-	expression tag	UNP P69706
B	42	GLY	-	expression tag	UNP P69706
B	43	GLY	-	expression tag	UNP P69706
B	44	GLY	-	expression tag	UNP P69706
B	45	TYR	-	expression tag	UNP P69706
B	46	TYR	-	expression tag	UNP P69706
B	47	TYR	-	expression tag	UNP P69706
B	48	TYR	-	expression tag	UNP P69706
B	49	TYR	-	expression tag	UNP P69706
B	50	TYR	-	expression tag	UNP P69706
B	128	LEU	-	linker	UNP P69706
B	129	GLU	-	linker	UNP P69706
B	130	VAL	ALA	engineered mutation	UNP P38507
B	138	MET	GLN	engineered mutation	UNP P38507
B	139	TRP	GLN	engineered mutation	UNP P38507
B	140	ALA	ASN	engineered mutation	UNP P38507
B	142	TRP	PHE	engineered mutation	UNP P38507
B	143	GLU	TYR	engineered mutation	UNP P38507
B	146	ARG	LEU	engineered mutation	UNP P38507
B	147	ASN	HIS	engineered mutation	UNP P38507
B	153	GLY	GLU	engineered mutation	UNP P38507
B	154	TRP	GLU	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
B	156	MET	ARG	engineered mutation	UNP P38507
B	157	THR	ASN	engineered mutation	UNP P38507
B	158	ALA	GLY	engineered mutation	UNP P38507
B	161	ALA	GLN	engineered mutation	UNP P38507
B	164	VAL	LYS	engineered mutation	UNP P38507
B	188	GLU	-	linker	UNP P38507
B	189	PHE	-	linker	UNP P38507
B	190	VAL	ALA	engineered mutation	UNP P38507
B	198	MET	GLN	engineered mutation	UNP P38507
B	199	TRP	GLN	engineered mutation	UNP P38507
B	200	ALA	ASN	engineered mutation	UNP P38507
B	202	TRP	PHE	engineered mutation	UNP P38507
B	203	GLU	TYR	engineered mutation	UNP P38507
B	206	ARG	LEU	engineered mutation	UNP P38507
B	207	ASN	HIS	engineered mutation	UNP P38507
B	213	GLY	GLU	engineered mutation	UNP P38507
B	214	TRP	GLU	engineered mutation	UNP P38507
B	216	MET	ARG	engineered mutation	UNP P38507
B	217	THR	ASN	engineered mutation	UNP P38507
B	218	ALA	GLY	engineered mutation	UNP P38507
B	221	ALA	GLN	engineered mutation	UNP P38507
B	224	VAL	LYS	engineered mutation	UNP P38507
B	248	GLY	-	linker	UNP P38507
B	249	SER	-	linker	UNP P38507
D	1	MET	-	initiating methionine	UNP P69706
D	2	HIS	-	expression tag	UNP P69706
D	3	HIS	-	expression tag	UNP P69706
D	4	HIS	-	expression tag	UNP P69706
D	5	HIS	-	expression tag	UNP P69706
D	6	HIS	-	expression tag	UNP P69706
D	7	HIS	-	expression tag	UNP P69706
D	8	MET	-	expression tag	UNP P69706
D	9	ALA	-	expression tag	UNP P69706
D	10	SER	-	expression tag	UNP P69706
D	11	SER	-	expression tag	UNP P69706
D	12	LEU	-	expression tag	UNP P69706
D	13	ARG	-	expression tag	UNP P69706
D	14	GLN	-	expression tag	UNP P69706
D	15	ILE	-	expression tag	UNP P69706
D	16	LEU	-	expression tag	UNP P69706
D	17	ASP	-	expression tag	UNP P69706
D	18	SER	-	expression tag	UNP P69706

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	GLN	-	expression tag	UNP P69706
D	20	LYS	-	expression tag	UNP P69706
D	21	MET	-	expression tag	UNP P69706
D	22	GLU	-	expression tag	UNP P69706
D	23	TRP	-	expression tag	UNP P69706
D	24	ARG	-	expression tag	UNP P69706
D	25	SER	-	expression tag	UNP P69706
D	26	ASN	-	expression tag	UNP P69706
D	27	ALA	-	expression tag	UNP P69706
D	28	GLY	-	expression tag	UNP P69706
D	29	GLY	-	expression tag	UNP P69706
D	30	SER	-	expression tag	UNP P69706
D	31	GLY	-	expression tag	UNP P69706
D	32	GLY	-	expression tag	UNP P69706
D	33	GLY	-	expression tag	UNP P69706
D	34	SER	-	expression tag	UNP P69706
D	35	GLY	-	expression tag	UNP P69706
D	36	GLY	-	expression tag	UNP P69706
D	37	GLY	-	expression tag	UNP P69706
D	38	THR	-	expression tag	UNP P69706
D	39	GLY	-	expression tag	UNP P69706
D	40	GLY	-	expression tag	UNP P69706
D	41	GLY	-	expression tag	UNP P69706
D	42	GLY	-	expression tag	UNP P69706
D	43	GLY	-	expression tag	UNP P69706
D	44	GLY	-	expression tag	UNP P69706
D	45	TYR	-	expression tag	UNP P69706
D	46	TYR	-	expression tag	UNP P69706
D	47	TYR	-	expression tag	UNP P69706
D	48	TYR	-	expression tag	UNP P69706
D	49	TYR	-	expression tag	UNP P69706
D	50	TYR	-	expression tag	UNP P69706
D	128	LEU	-	linker	UNP P69706
D	129	GLU	-	linker	UNP P69706
D	130	VAL	ALA	engineered mutation	UNP P38507
D	138	MET	GLN	engineered mutation	UNP P38507
D	139	TRP	GLN	engineered mutation	UNP P38507
D	140	ALA	ASN	engineered mutation	UNP P38507
D	142	TRP	PHE	engineered mutation	UNP P38507
D	143	GLU	TYR	engineered mutation	UNP P38507
D	146	ARG	LEU	engineered mutation	UNP P38507
D	147	ASN	HIS	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
D	153	GLY	GLU	engineered mutation	UNP P38507
D	154	TRP	GLU	engineered mutation	UNP P38507
D	156	MET	ARG	engineered mutation	UNP P38507
D	157	THR	ASN	engineered mutation	UNP P38507
D	158	ALA	GLY	engineered mutation	UNP P38507
D	161	ALA	GLN	engineered mutation	UNP P38507
D	164	VAL	LYS	engineered mutation	UNP P38507
D	188	GLU	-	linker	UNP P38507
D	189	PHE	-	linker	UNP P38507
D	190	VAL	ALA	engineered mutation	UNP P38507
D	198	MET	GLN	engineered mutation	UNP P38507
D	199	TRP	GLN	engineered mutation	UNP P38507
D	200	ALA	ASN	engineered mutation	UNP P38507
D	202	TRP	PHE	engineered mutation	UNP P38507
D	203	GLU	TYR	engineered mutation	UNP P38507
D	206	ARG	LEU	engineered mutation	UNP P38507
D	207	ASN	HIS	engineered mutation	UNP P38507
D	213	GLY	GLU	engineered mutation	UNP P38507
D	214	TRP	GLU	engineered mutation	UNP P38507
D	216	MET	ARG	engineered mutation	UNP P38507
D	217	THR	ASN	engineered mutation	UNP P38507
D	218	ALA	GLY	engineered mutation	UNP P38507
D	221	ALA	GLN	engineered mutation	UNP P38507
D	224	VAL	LYS	engineered mutation	UNP P38507
D	248	GLY	-	linker	UNP P38507
D	249	SER	-	linker	UNP P38507
C	1	MET	-	initiating methionine	UNP P69706
C	2	HIS	-	expression tag	UNP P69706
C	3	HIS	-	expression tag	UNP P69706
C	4	HIS	-	expression tag	UNP P69706
C	5	HIS	-	expression tag	UNP P69706
C	6	HIS	-	expression tag	UNP P69706
C	7	HIS	-	expression tag	UNP P69706
C	8	MET	-	expression tag	UNP P69706
C	9	ALA	-	expression tag	UNP P69706
C	10	SER	-	expression tag	UNP P69706
C	11	SER	-	expression tag	UNP P69706
C	12	LEU	-	expression tag	UNP P69706
C	13	ARG	-	expression tag	UNP P69706
C	14	GLN	-	expression tag	UNP P69706
C	15	ILE	-	expression tag	UNP P69706
C	16	LEU	-	expression tag	UNP P69706

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	ASP	-	expression tag	UNP P69706
C	18	SER	-	expression tag	UNP P69706
C	19	GLN	-	expression tag	UNP P69706
C	20	LYS	-	expression tag	UNP P69706
C	21	MET	-	expression tag	UNP P69706
C	22	GLU	-	expression tag	UNP P69706
C	23	TRP	-	expression tag	UNP P69706
C	24	ARG	-	expression tag	UNP P69706
C	25	SER	-	expression tag	UNP P69706
C	26	ASN	-	expression tag	UNP P69706
C	27	ALA	-	expression tag	UNP P69706
C	28	GLY	-	expression tag	UNP P69706
C	29	GLY	-	expression tag	UNP P69706
C	30	SER	-	expression tag	UNP P69706
C	31	GLY	-	expression tag	UNP P69706
C	32	GLY	-	expression tag	UNP P69706
C	33	GLY	-	expression tag	UNP P69706
C	34	SER	-	expression tag	UNP P69706
C	35	GLY	-	expression tag	UNP P69706
C	36	GLY	-	expression tag	UNP P69706
C	37	GLY	-	expression tag	UNP P69706
C	38	THR	-	expression tag	UNP P69706
C	39	GLY	-	expression tag	UNP P69706
C	40	GLY	-	expression tag	UNP P69706
C	41	GLY	-	expression tag	UNP P69706
C	42	GLY	-	expression tag	UNP P69706
C	43	GLY	-	expression tag	UNP P69706
C	44	GLY	-	expression tag	UNP P69706
C	45	TYR	-	expression tag	UNP P69706
C	46	TYR	-	expression tag	UNP P69706
C	47	TYR	-	expression tag	UNP P69706
C	48	TYR	-	expression tag	UNP P69706
C	49	TYR	-	expression tag	UNP P69706
C	50	TYR	-	expression tag	UNP P69706
C	128	LEU	-	linker	UNP P69706
C	129	GLU	-	linker	UNP P69706
C	130	VAL	ALA	engineered mutation	UNP P38507
C	138	MET	GLN	engineered mutation	UNP P38507
C	139	TRP	GLN	engineered mutation	UNP P38507
C	140	ALA	ASN	engineered mutation	UNP P38507
C	142	TRP	PHE	engineered mutation	UNP P38507
C	143	GLU	TYR	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
C	146	ARG	LEU	engineered mutation	UNP P38507
C	147	ASN	HIS	engineered mutation	UNP P38507
C	153	GLY	GLU	engineered mutation	UNP P38507
C	154	TRP	GLU	engineered mutation	UNP P38507
C	156	MET	ARG	engineered mutation	UNP P38507
C	157	THR	ASN	engineered mutation	UNP P38507
C	158	ALA	GLY	engineered mutation	UNP P38507
C	161	ALA	GLN	engineered mutation	UNP P38507
C	164	VAL	LYS	engineered mutation	UNP P38507
C	188	GLU	-	linker	UNP P38507
C	189	PHE	-	linker	UNP P38507
C	190	VAL	ALA	engineered mutation	UNP P38507
C	198	MET	GLN	engineered mutation	UNP P38507
C	199	TRP	GLN	engineered mutation	UNP P38507
C	200	ALA	ASN	engineered mutation	UNP P38507
C	202	TRP	PHE	engineered mutation	UNP P38507
C	203	GLU	TYR	engineered mutation	UNP P38507
C	206	ARG	LEU	engineered mutation	UNP P38507
C	207	ASN	HIS	engineered mutation	UNP P38507
C	213	GLY	GLU	engineered mutation	UNP P38507
C	214	TRP	GLU	engineered mutation	UNP P38507
C	216	MET	ARG	engineered mutation	UNP P38507
C	217	THR	ASN	engineered mutation	UNP P38507
C	218	ALA	GLY	engineered mutation	UNP P38507
C	221	ALA	GLN	engineered mutation	UNP P38507
C	224	VAL	LYS	engineered mutation	UNP P38507
C	248	GLY	-	linker	UNP P38507
C	249	SER	-	linker	UNP P38507

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.902	Depositor
Minimum map value	-0.612	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	840.0, 840.0, 840.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1138	0.46	0/1556
1	B	0.28	0/1138	0.48	0/1556
1	C	0.28	0/1138	0.55	0/1556
1	D	0.27	0/1138	0.52	0/1556
All	All	0.27	0/4552	0.50	0/6224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1104	0	1082	28	0
1	B	1104	0	1082	17	0
1	C	1104	0	1082	44	0
1	D	1104	0	1082	27	0
All	All	4416	0	4328	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:VAL:HG12	1:C:259:ASN:HD22	1.45	0.81
1:A:65:LEU:HD12	1:A:268:GLN:HG3	1.63	0.80
1:B:276:CYS:HB2	1:B:281:ARG:HG3	1.66	0.77
1:C:74:PRO:HG2	1:C:79:LEU:HD21	1.68	0.73
1:C:87:TYR:HB3	1:C:90:ALA:HB3	1.72	0.71

There are no symmetry-related clashes.

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	Percentiles	
1	A	133/318 (42%)	130 (98%)	3 (2%)	0	100	100
1	B	133/318 (42%)	127 (96%)	6 (4%)	0	100	100
1	C	133/318 (42%)	125 (94%)	8 (6%)	0	100	100
1	D	133/318 (42%)	125 (94%)	8 (6%)	0	100	100
All	All	532/1272 (42%)	507 (95%)	25 (5%)	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	Percentiles	
1	A	122/266 (46%)	122 (100%)	0	100	100
1	B	122/266 (46%)	122 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	122/266 (46%)	122 (100%)	0	100	100
1	D	122/266 (46%)	122 (100%)	0	100	100
All	All	488/1064 (46%)	488 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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.

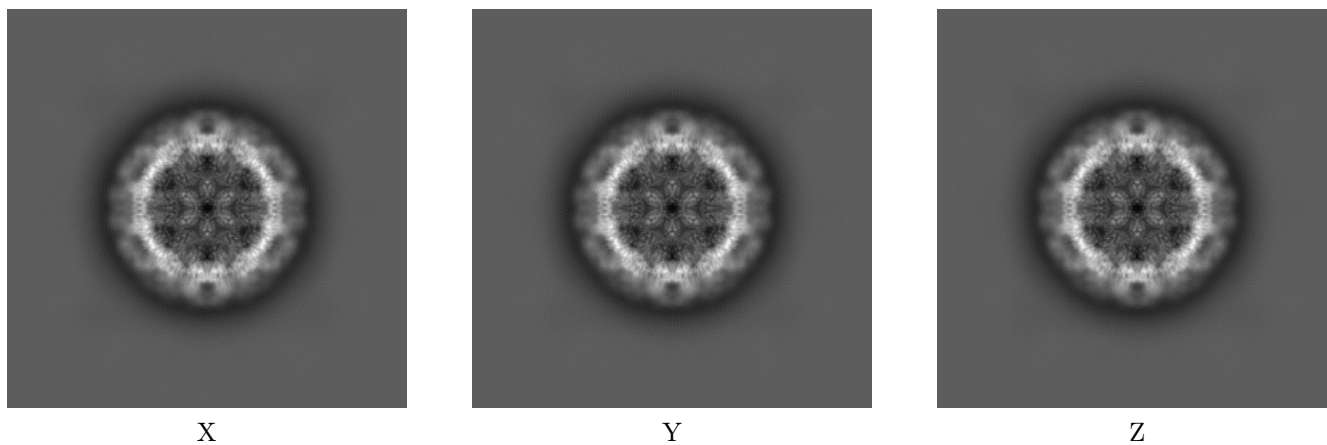
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31545. 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.

6.1 Orthogonal projections [i](#)

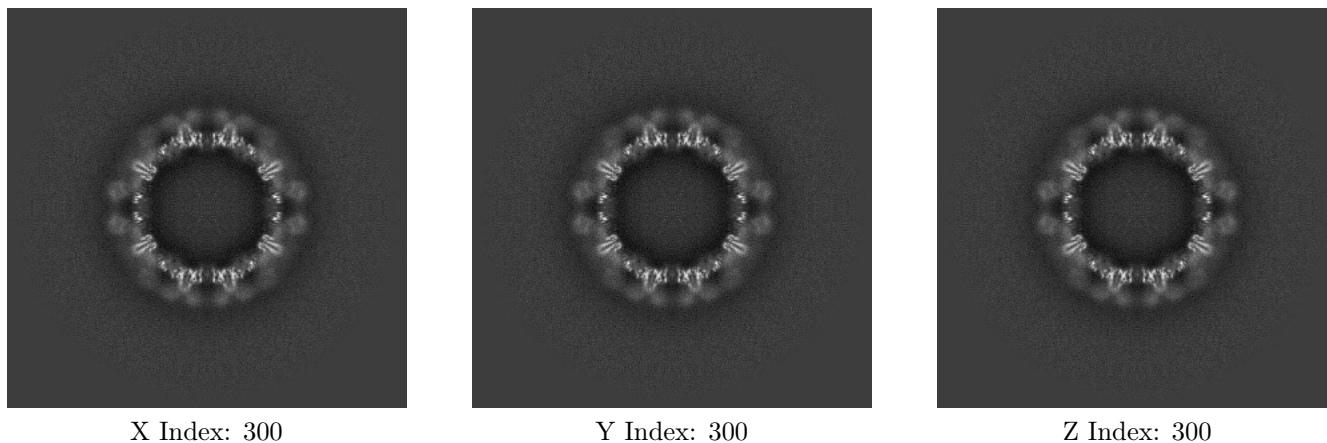
6.1.1 Primary map



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

6.2 Central slices [i](#)

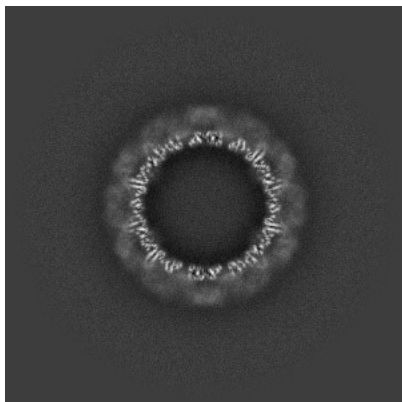
6.2.1 Primary map



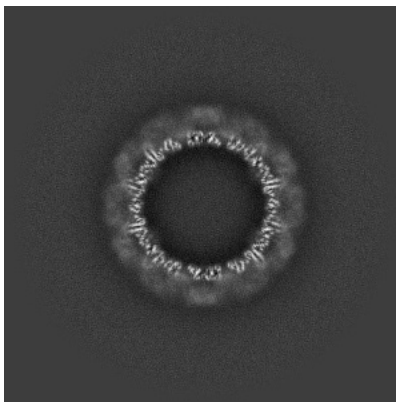
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

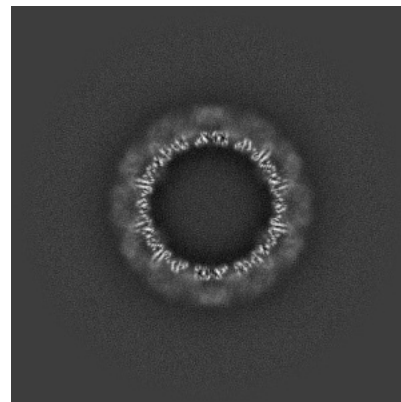
6.3.1 Primary map



X Index: 280



Y Index: 320

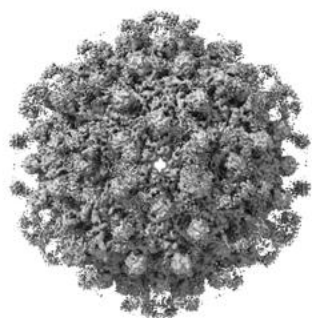


Z Index: 280

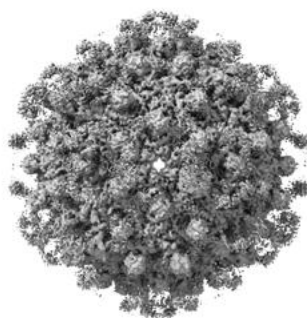
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

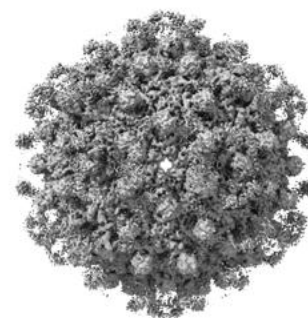
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

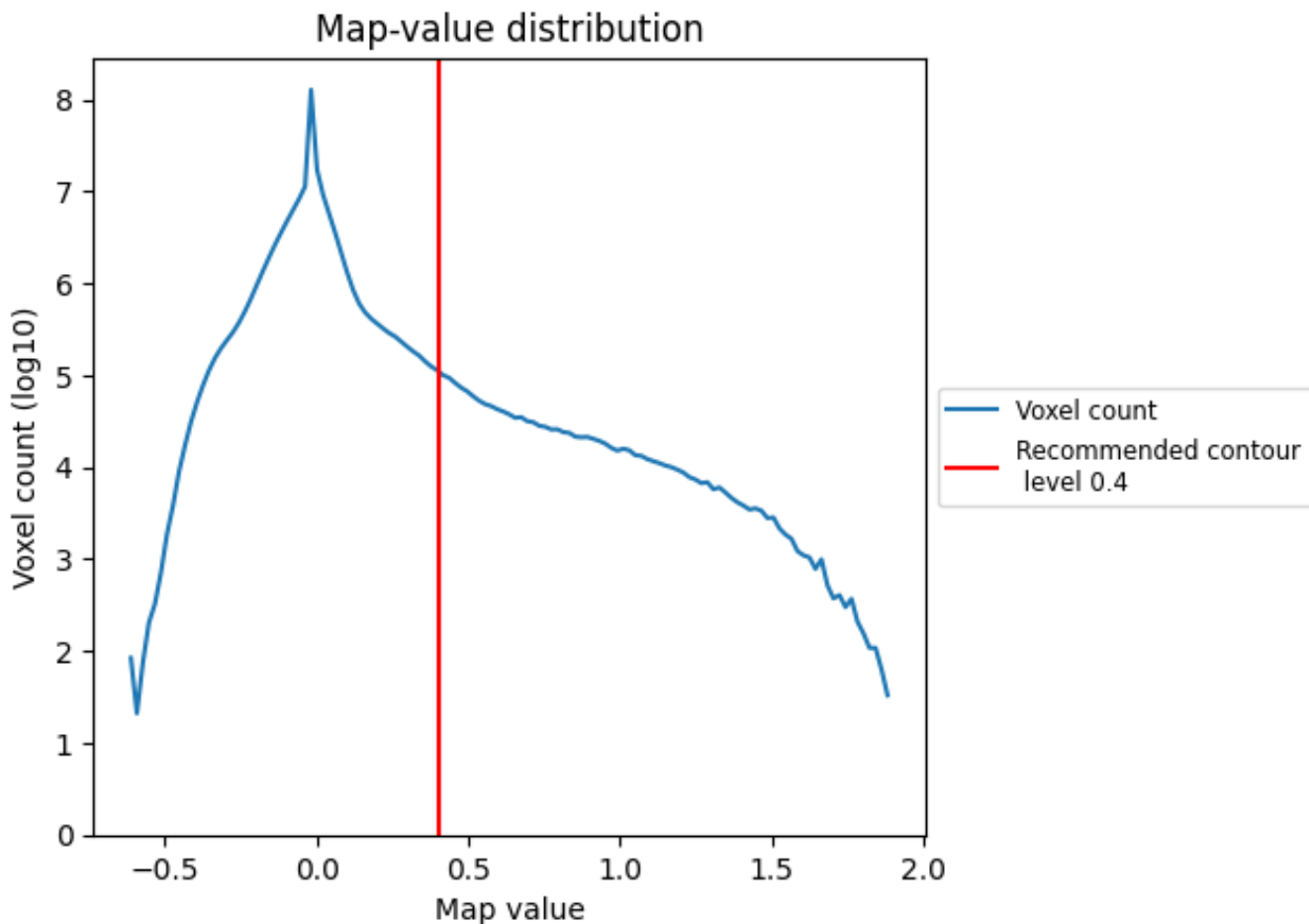
6.5 Mask visualisation

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

7 Map analysis [i](#)

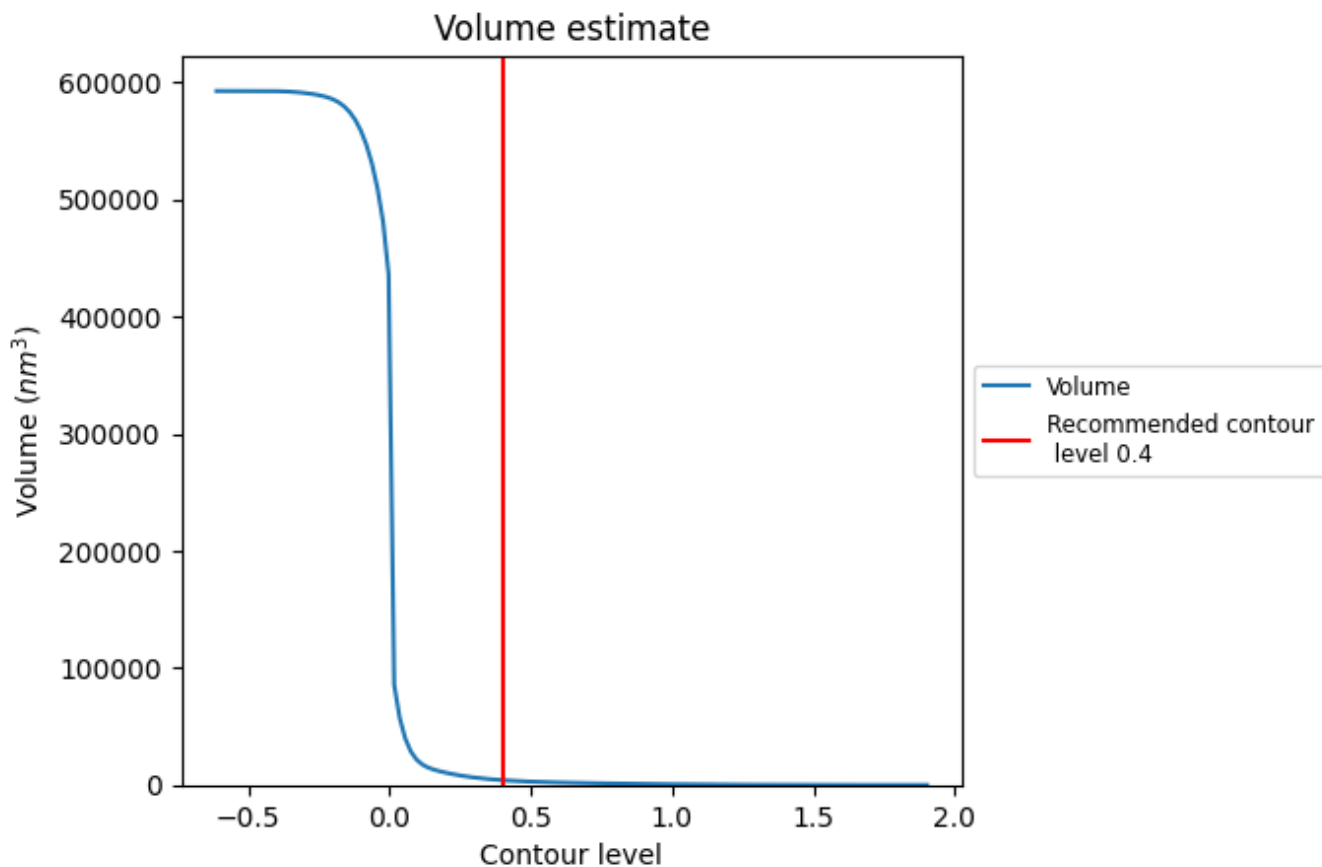
This section contains the results of statistical analysis of the map.

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.

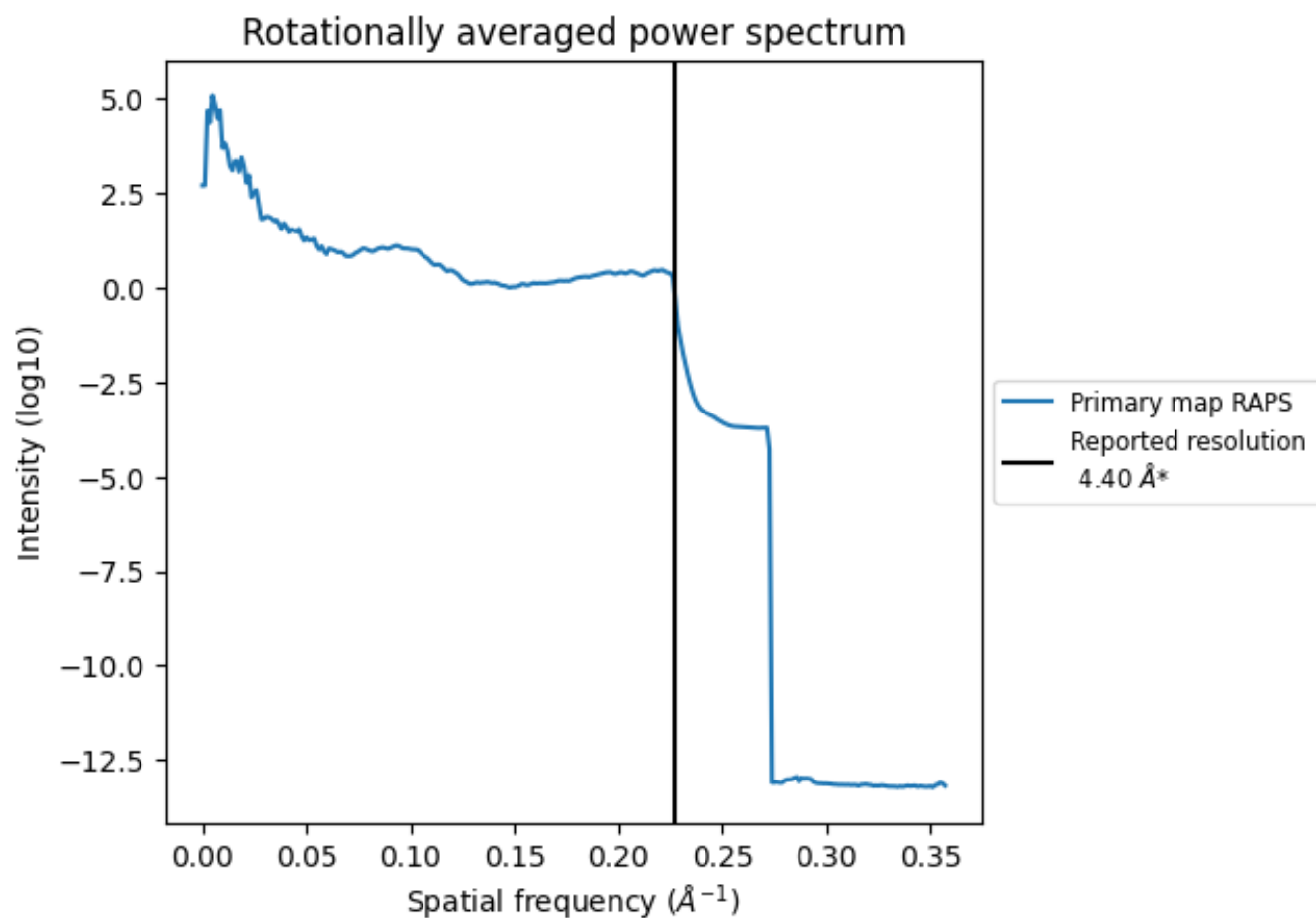
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 4113 nm³; this corresponds to an approximate mass of 3715 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 0.227\AA^{-1}

8 Fourier-Shell correlation

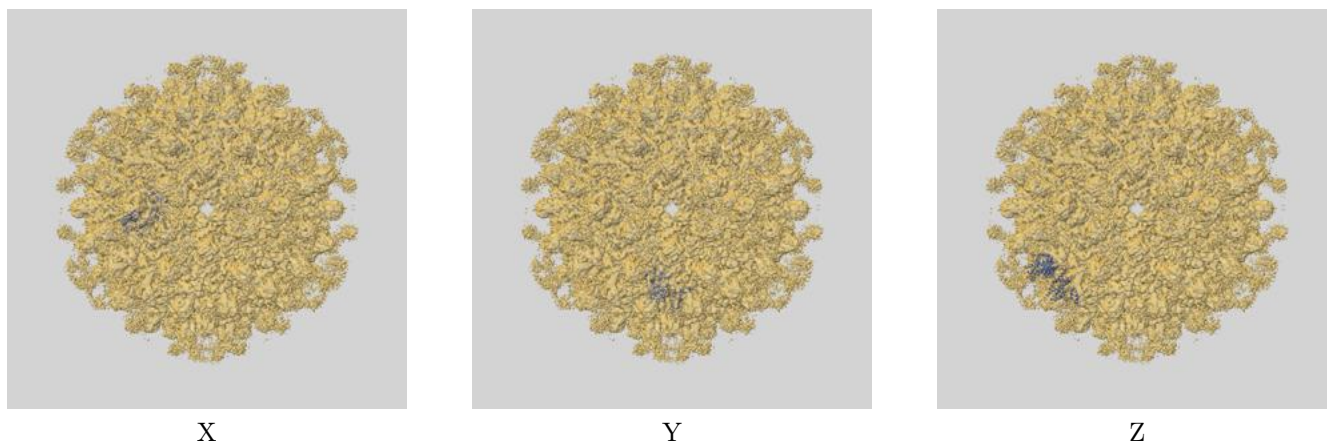
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

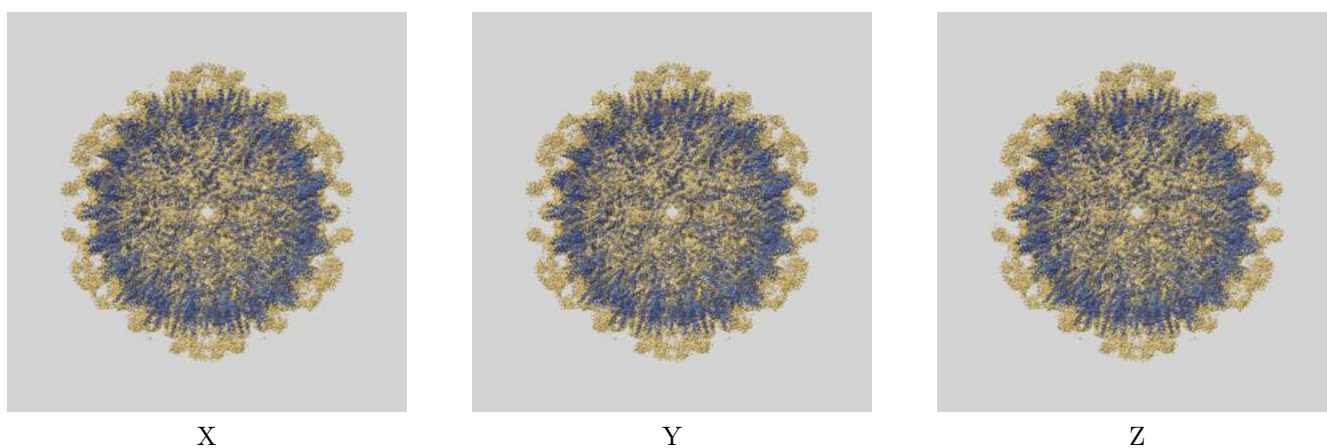
This section contains information regarding the fit between EMDB map EMD-31545 and PDB model 7FDJ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

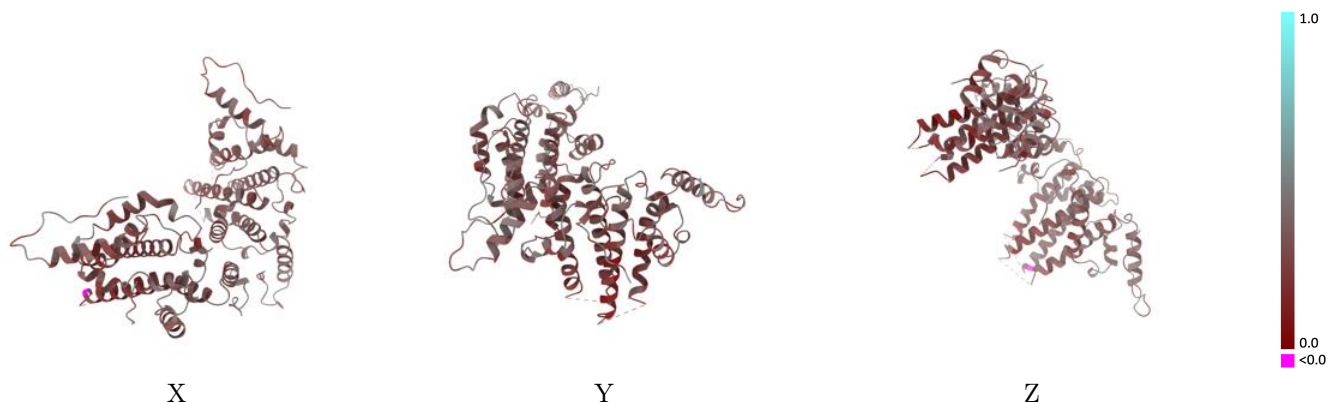


9.1.2 Map-model assembly overlay [i](#)



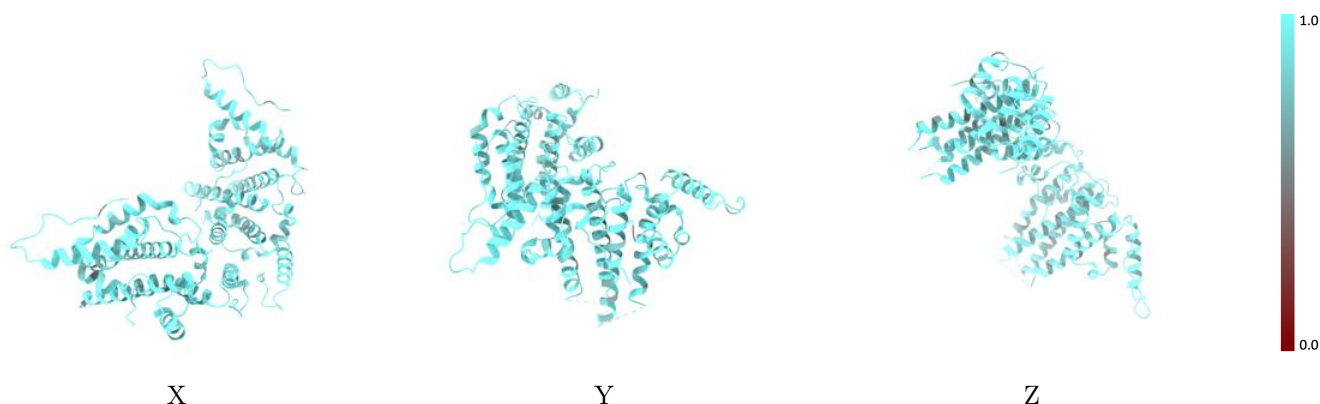
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



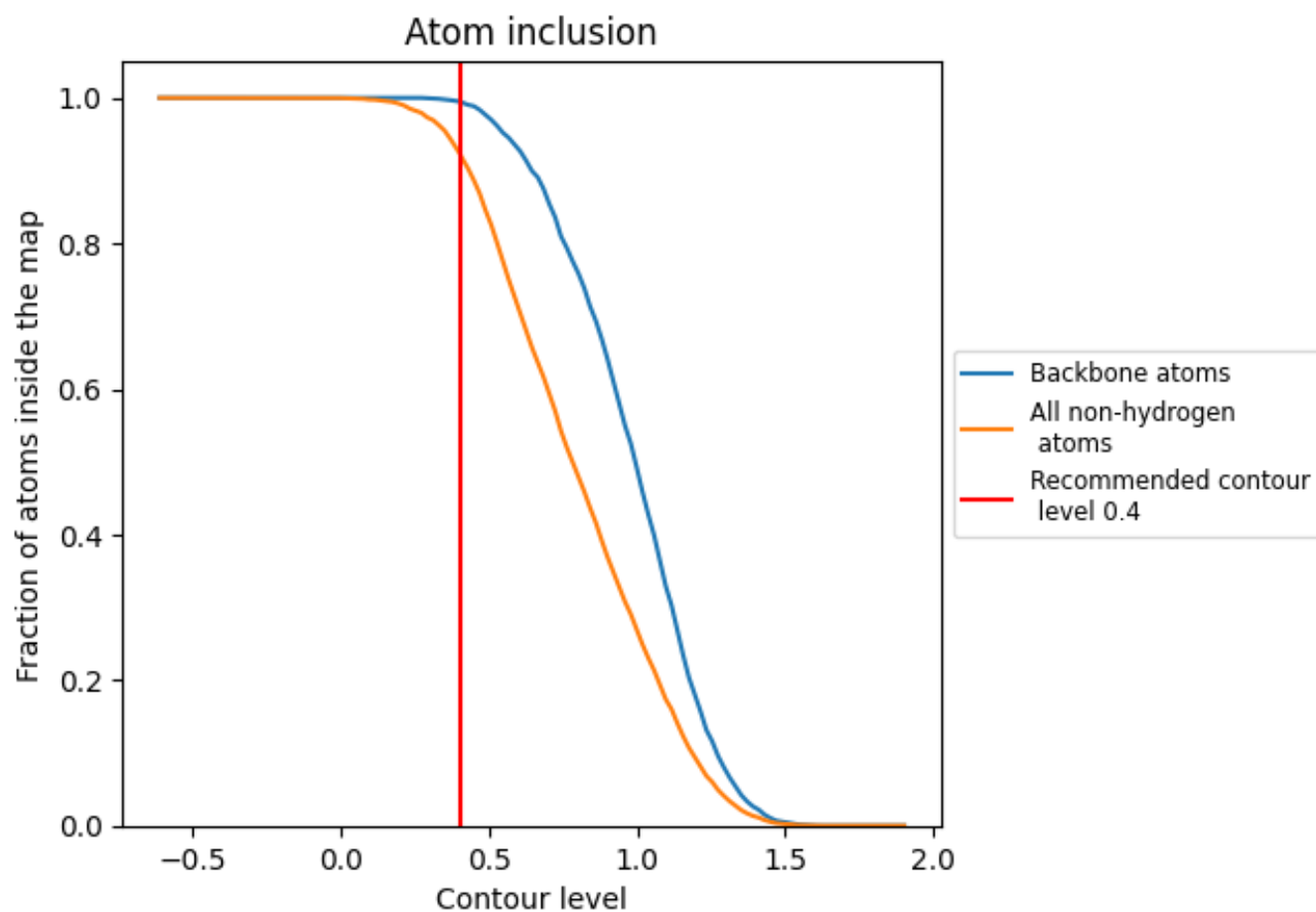
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).



9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9242	 0.3120
A	 0.9259	 0.3010
B	 0.9370	 0.3240
C	 0.9342	 0.3210
D	 0.8999	 0.3010

