wwPDB EM Validation Summary Report

Mar 19, 2026 – 10:54 PM UTC

PDB ID	:	7EP6 / pdb_00007ep6
EMDB ID	:	EMD-31234
Title	:	Engineered Hepatitis B virus core antigen T=4
Authors	:	Jeong, H.; Heo, Y.; Yoo, Y.; Ryu, B.; Yun, J.; Cho, H.; Lee, W.
Deposited on	:	2021-04-26
Resolution	:	3.86 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:

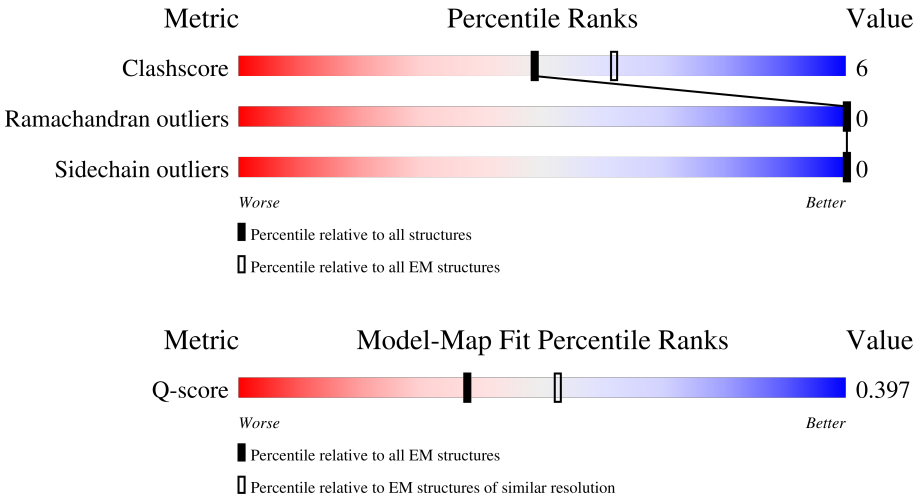
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.86 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8889 (3.36 - 4.35)

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	A	337	5% 34% 8% 58%
1	B	337	6% 34% 7% 58%
1	C	337	6% 36% 5% 58%
1	D	337	5% 37% • 58%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4536 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
1	A	141	Total	C	N	O	S	0	0
			1134	738	186	205	5		
1	B	141	Total	C	N	O	S	0	0
			1134	738	186	205	5		
1	C	141	Total	C	N	O	S	0	0
			1134	738	186	205	5		
1	D	141	Total	C	N	O	S	0	0
			1134	738	186	205	5		

There are 420 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

Continued on next page...

Continued from previous page...

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	138	GLY	-	linker	UNP P69706
A	139	GLY	-	linker	UNP P69706
A	140	GLY	-	linker	UNP P69706
A	141	GLY	-	linker	UNP P69706
A	142	SER	-	linker	UNP P69706
A	143	GLY	-	linker	UNP P69706
A	144	GLY	-	linker	UNP P69706
A	145	GLY	-	linker	UNP P69706
A	146	GLY	-	linker	UNP P69706
A	147	THR	-	linker	UNP P69706
A	148	LEU	-	linker	UNP P69706
A	149	GLU	-	linker	UNP P69706
A	150	VAL	ALA	engineered mutation	UNP P38507
A	158	MET	GLN	engineered mutation	UNP P38507

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	TRP	GLN	engineered mutation	UNP P38507
A	160	ALA	ASN	engineered mutation	UNP P38507
A	162	TRP	PHE	engineered mutation	UNP P38507
A	163	GLU	TYR	engineered mutation	UNP P38507
A	166	ARG	LEU	engineered mutation	UNP P38507
A	167	ASN	HIS	engineered mutation	UNP P38507
A	173	GLY	GLU	engineered mutation	UNP P38507
A	174	TRP	GLU	engineered mutation	UNP P38507
A	176	MET	ARG	engineered mutation	UNP P38507
A	177	THR	ASN	engineered mutation	UNP P38507
A	178	ALA	GLY	engineered mutation	UNP P38507
A	181	ALA	GLN	engineered mutation	UNP P38507
A	184	VAL	LYS	engineered mutation	UNP P38507
A	208	GLU	-	linker	UNP P38507
A	209	PHE	-	linker	UNP P38507
A	210	VAL	ALA	engineered mutation	UNP P38507
A	218	MET	GLN	engineered mutation	UNP P38507
A	219	TRP	GLN	engineered mutation	UNP P38507
A	220	ALA	ASN	engineered mutation	UNP P38507
A	222	TRP	PHE	engineered mutation	UNP P38507
A	223	GLU	TYR	engineered mutation	UNP P38507
A	226	ARG	LEU	engineered mutation	UNP P38507
A	227	ASN	HIS	engineered mutation	UNP P38507
A	233	GLY	GLU	engineered mutation	UNP P38507
A	234	TRP	GLU	engineered mutation	UNP P38507
A	236	MET	ARG	engineered mutation	UNP P38507
A	237	THR	ASN	engineered mutation	UNP P38507
A	238	ALA	GLY	engineered mutation	UNP P38507
A	241	ALA	GLN	engineered mutation	UNP P38507
A	244	VAL	LYS	engineered mutation	UNP P38507
A	268	GLY	-	linker	UNP P38507
A	269	SER	-	linker	UNP P38507
A	270	GLY	-	linker	UNP P38507
A	271	GLY	-	linker	UNP P38507
A	272	GLY	-	linker	UNP P38507
A	273	GLY	-	linker	UNP P38507
A	274	SER	-	linker	UNP P38507
A	275	GLY	-	linker	UNP P38507
A	276	GLY	-	linker	UNP P38507
A	277	GLY	-	linker	UNP P38507
A	278	GLY	-	linker	UNP P38507
B	1	MET	-	initiating methionine	UNP P69706

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	138	GLY	-	linker	UNP P69706
B	139	GLY	-	linker	UNP P69706
B	140	GLY	-	linker	UNP P69706
B	141	GLY	-	linker	UNP P69706
B	142	SER	-	linker	UNP P69706
B	143	GLY	-	linker	UNP P69706
B	144	GLY	-	linker	UNP P69706
B	145	GLY	-	linker	UNP P69706
B	146	GLY	-	linker	UNP P69706
B	147	THR	-	linker	UNP P69706
B	148	LEU	-	linker	UNP P69706
B	149	GLU	-	linker	UNP P69706
B	150	VAL	ALA	engineered mutation	UNP P38507
B	158	MET	GLN	engineered mutation	UNP P38507
B	159	TRP	GLN	engineered mutation	UNP P38507
B	160	ALA	ASN	engineered mutation	UNP P38507
B	162	TRP	PHE	engineered mutation	UNP P38507
B	163	GLU	TYR	engineered mutation	UNP P38507
B	166	ARG	LEU	engineered mutation	UNP P38507
B	167	ASN	HIS	engineered mutation	UNP P38507
B	173	GLY	GLU	engineered mutation	UNP P38507
B	174	TRP	GLU	engineered mutation	UNP P38507
B	176	MET	ARG	engineered mutation	UNP P38507
B	177	THR	ASN	engineered mutation	UNP P38507
B	178	ALA	GLY	engineered mutation	UNP P38507
B	181	ALA	GLN	engineered mutation	UNP P38507
B	184	VAL	LYS	engineered mutation	UNP P38507
B	208	GLU	-	linker	UNP P38507
B	209	PHE	-	linker	UNP P38507
B	210	VAL	ALA	engineered mutation	UNP P38507
B	218	MET	GLN	engineered mutation	UNP P38507
B	219	TRP	GLN	engineered mutation	UNP P38507
B	220	ALA	ASN	engineered mutation	UNP P38507
B	222	TRP	PHE	engineered mutation	UNP P38507
B	223	GLU	TYR	engineered mutation	UNP P38507

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	226	ARG	LEU	engineered mutation	UNP P38507
B	227	ASN	HIS	engineered mutation	UNP P38507
B	233	GLY	GLU	engineered mutation	UNP P38507
B	234	TRP	GLU	engineered mutation	UNP P38507
B	236	MET	ARG	engineered mutation	UNP P38507
B	237	THR	ASN	engineered mutation	UNP P38507
B	238	ALA	GLY	engineered mutation	UNP P38507
B	241	ALA	GLN	engineered mutation	UNP P38507
B	244	VAL	LYS	engineered mutation	UNP P38507
B	268	GLY	-	linker	UNP P38507
B	269	SER	-	linker	UNP P38507
B	270	GLY	-	linker	UNP P38507
B	271	GLY	-	linker	UNP P38507
B	272	GLY	-	linker	UNP P38507
B	273	GLY	-	linker	UNP P38507
B	274	SER	-	linker	UNP P38507
B	275	GLY	-	linker	UNP P38507
B	276	GLY	-	linker	UNP P38507
B	277	GLY	-	linker	UNP P38507
B	278	GLY	-	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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	138	GLY	-	linker	UNP P69706
C	139	GLY	-	linker	UNP P69706
C	140	GLY	-	linker	UNP P69706
C	141	GLY	-	linker	UNP P69706
C	142	SER	-	linker	UNP P69706
C	143	GLY	-	linker	UNP P69706
C	144	GLY	-	linker	UNP P69706
C	145	GLY	-	linker	UNP P69706
C	146	GLY	-	linker	UNP P69706
C	147	THR	-	linker	UNP P69706
C	148	LEU	-	linker	UNP P69706
C	149	GLU	-	linker	UNP P69706
C	150	VAL	ALA	engineered mutation	UNP P38507
C	158	MET	GLN	engineered mutation	UNP P38507

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	159	TRP	GLN	engineered mutation	UNP P38507
C	160	ALA	ASN	engineered mutation	UNP P38507
C	162	TRP	PHE	engineered mutation	UNP P38507
C	163	GLU	TYR	engineered mutation	UNP P38507
C	166	ARG	LEU	engineered mutation	UNP P38507
C	167	ASN	HIS	engineered mutation	UNP P38507
C	173	GLY	GLU	engineered mutation	UNP P38507
C	174	TRP	GLU	engineered mutation	UNP P38507
C	176	MET	ARG	engineered mutation	UNP P38507
C	177	THR	ASN	engineered mutation	UNP P38507
C	178	ALA	GLY	engineered mutation	UNP P38507
C	181	ALA	GLN	engineered mutation	UNP P38507
C	184	VAL	LYS	engineered mutation	UNP P38507
C	208	GLU	-	linker	UNP P38507
C	209	PHE	-	linker	UNP P38507
C	210	VAL	ALA	engineered mutation	UNP P38507
C	218	MET	GLN	engineered mutation	UNP P38507
C	219	TRP	GLN	engineered mutation	UNP P38507
C	220	ALA	ASN	engineered mutation	UNP P38507
C	222	TRP	PHE	engineered mutation	UNP P38507
C	223	GLU	TYR	engineered mutation	UNP P38507
C	226	ARG	LEU	engineered mutation	UNP P38507
C	227	ASN	HIS	engineered mutation	UNP P38507
C	233	GLY	GLU	engineered mutation	UNP P38507
C	234	TRP	GLU	engineered mutation	UNP P38507
C	236	MET	ARG	engineered mutation	UNP P38507
C	237	THR	ASN	engineered mutation	UNP P38507
C	238	ALA	GLY	engineered mutation	UNP P38507
C	241	ALA	GLN	engineered mutation	UNP P38507
C	244	VAL	LYS	engineered mutation	UNP P38507
C	268	GLY	-	linker	UNP P38507
C	269	SER	-	linker	UNP P38507
C	270	GLY	-	linker	UNP P38507
C	271	GLY	-	linker	UNP P38507
C	272	GLY	-	linker	UNP P38507
C	273	GLY	-	linker	UNP P38507
C	274	SER	-	linker	UNP P38507
C	275	GLY	-	linker	UNP P38507
C	276	GLY	-	linker	UNP P38507
C	277	GLY	-	linker	UNP P38507
C	278	GLY	-	linker	UNP P38507
D	1	MET	-	initiating methionine	UNP P69706

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	138	GLY	-	linker	UNP P69706
D	139	GLY	-	linker	UNP P69706
D	140	GLY	-	linker	UNP P69706
D	141	GLY	-	linker	UNP P69706
D	142	SER	-	linker	UNP P69706
D	143	GLY	-	linker	UNP P69706
D	144	GLY	-	linker	UNP P69706
D	145	GLY	-	linker	UNP P69706
D	146	GLY	-	linker	UNP P69706
D	147	THR	-	linker	UNP P69706
D	148	LEU	-	linker	UNP P69706
D	149	GLU	-	linker	UNP P69706
D	150	VAL	ALA	engineered mutation	UNP P38507
D	158	MET	GLN	engineered mutation	UNP P38507
D	159	TRP	GLN	engineered mutation	UNP P38507
D	160	ALA	ASN	engineered mutation	UNP P38507
D	162	TRP	PHE	engineered mutation	UNP P38507
D	163	GLU	TYR	engineered mutation	UNP P38507
D	166	ARG	LEU	engineered mutation	UNP P38507
D	167	ASN	HIS	engineered mutation	UNP P38507
D	173	GLY	GLU	engineered mutation	UNP P38507
D	174	TRP	GLU	engineered mutation	UNP P38507
D	176	MET	ARG	engineered mutation	UNP P38507
D	177	THR	ASN	engineered mutation	UNP P38507
D	178	ALA	GLY	engineered mutation	UNP P38507
D	181	ALA	GLN	engineered mutation	UNP P38507
D	184	VAL	LYS	engineered mutation	UNP P38507
D	208	GLU	-	linker	UNP P38507
D	209	PHE	-	linker	UNP P38507
D	210	VAL	ALA	engineered mutation	UNP P38507
D	218	MET	GLN	engineered mutation	UNP P38507
D	219	TRP	GLN	engineered mutation	UNP P38507
D	220	ALA	ASN	engineered mutation	UNP P38507
D	222	TRP	PHE	engineered mutation	UNP P38507
D	223	GLU	TYR	engineered mutation	UNP P38507

Continued on next page...

Continued from previous page...

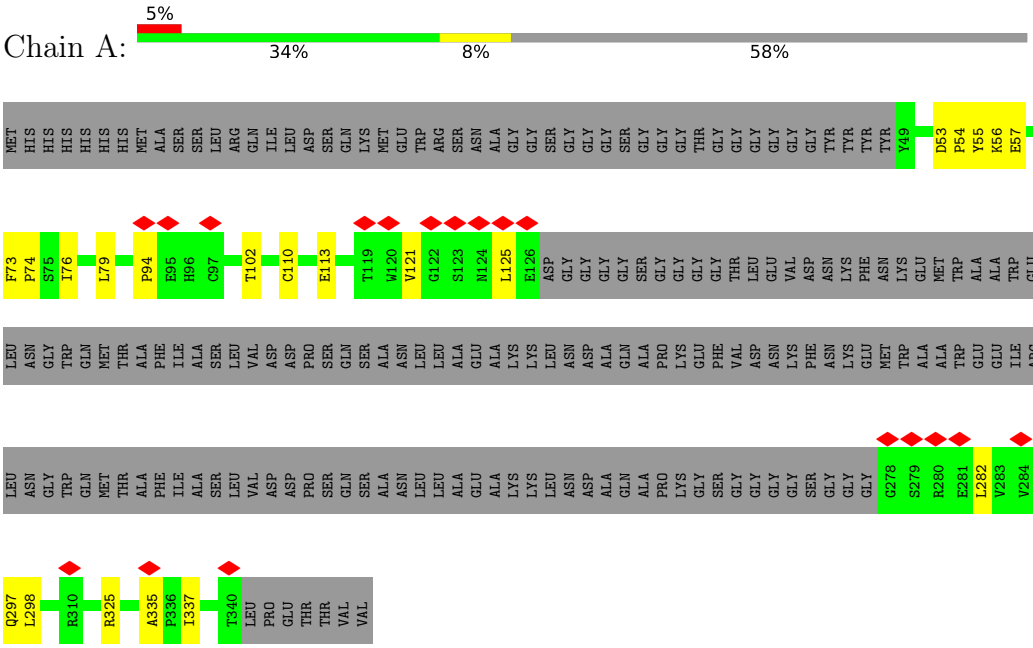
Chain	Residue	Modelled	Actual	Comment	Reference
D	226	ARG	LEU	engineered mutation	UNP P38507
D	227	ASN	HIS	engineered mutation	UNP P38507
D	233	GLY	GLU	engineered mutation	UNP P38507
D	234	TRP	GLU	engineered mutation	UNP P38507
D	236	MET	ARG	engineered mutation	UNP P38507
D	237	THR	ASN	engineered mutation	UNP P38507
D	238	ALA	GLY	engineered mutation	UNP P38507
D	241	ALA	GLN	engineered mutation	UNP P38507
D	244	VAL	LYS	engineered mutation	UNP P38507
D	268	GLY	-	linker	UNP P38507
D	269	SER	-	linker	UNP P38507
D	270	GLY	-	linker	UNP P38507
D	271	GLY	-	linker	UNP P38507
D	272	GLY	-	linker	UNP P38507
D	273	GLY	-	linker	UNP P38507
D	274	SER	-	linker	UNP P38507
D	275	GLY	-	linker	UNP P38507
D	276	GLY	-	linker	UNP P38507
D	277	GLY	-	linker	UNP P38507
D	278	GLY	-	linker	UNP P38507

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.

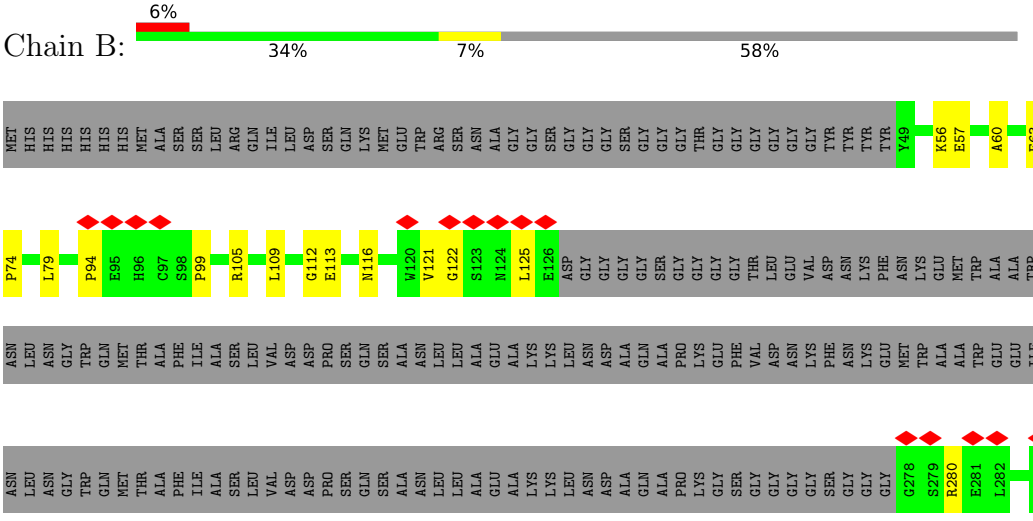
• Molecule 1: Capsid protein,Immunoglobulin G-binding protein A

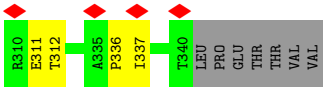
Chain A:



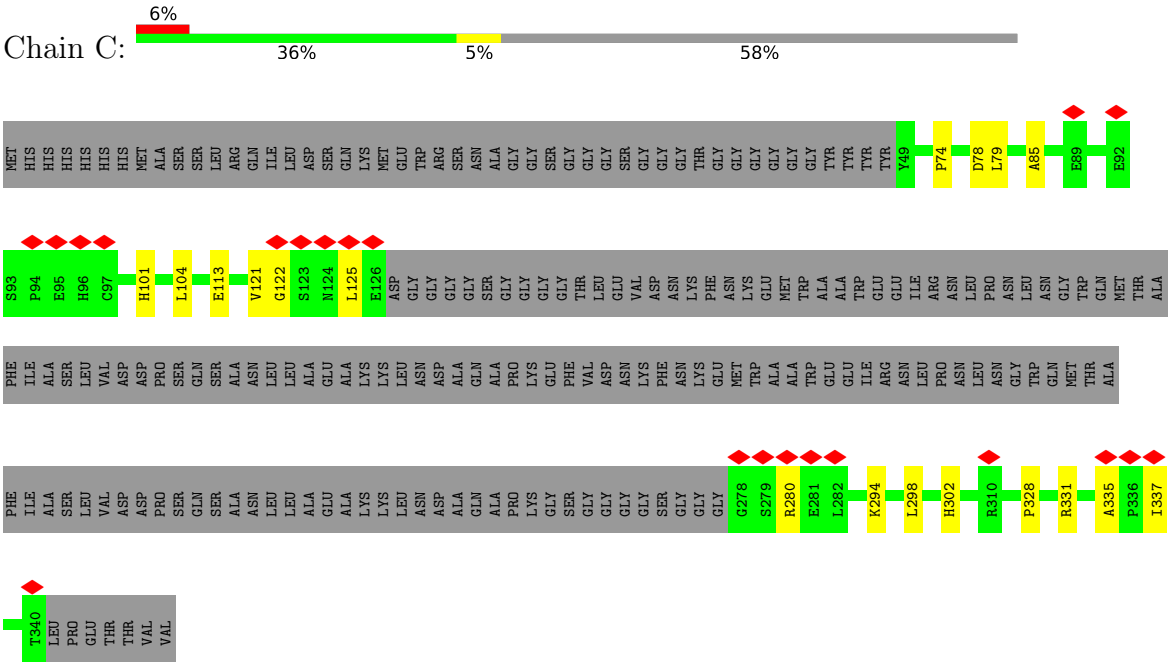
• Molecule 1: Capsid protein,Immunoglobulin G-binding protein A

Chain B:

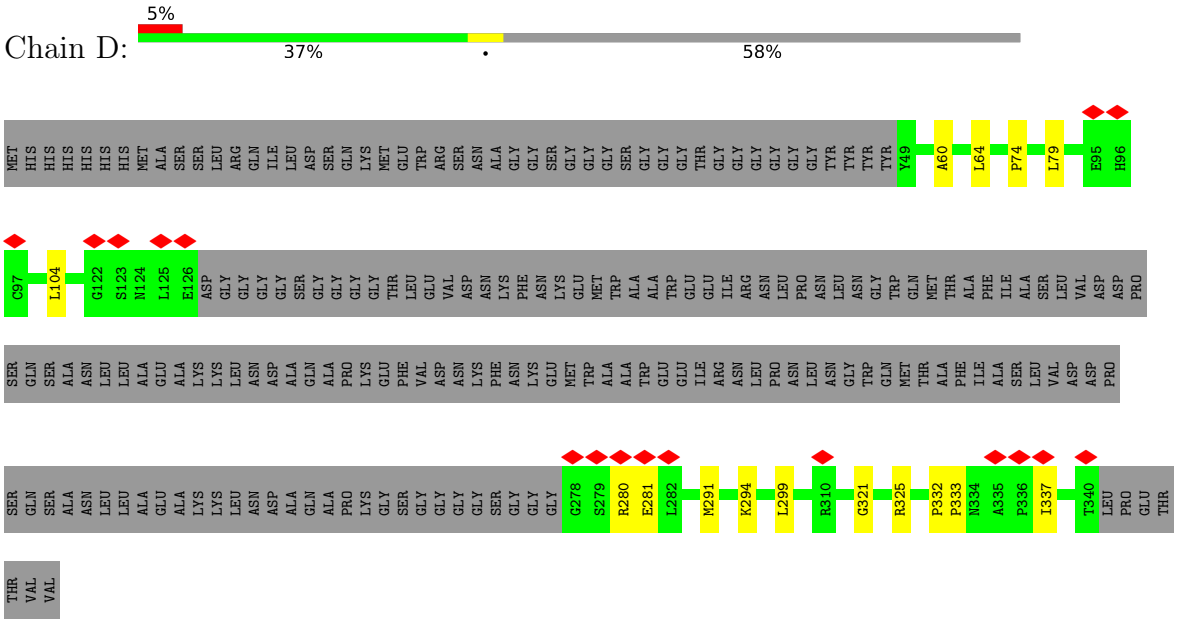




• Molecule 1: Capsid protein,Immunoglobulin G-binding protein A



• Molecule 1: Capsid protein,Immunoglobulin G-binding protein A



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68577	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 ($e^-/Å^2$)	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	2.648	Depositor
Minimum map value	-0.936	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.67	Depositor
Map size (Å)	630.0, 630.0, 630.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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	0.14	0/1168	0.33	0/1595
1	B	0.15	0/1168	0.42	1/1595 (0.1%)
1	C	0.15	0/1168	0.35	0/1595
1	D	0.15	0/1168	0.34	0/1595
All	All	0.15	0/4672	0.36	1/6380 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	336	PRO	CA-N-CD	-5.20	104.72	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1134	0	1108	21	0
1	B	1134	0	1108	20	0
1	C	1134	0	1108	12	0
1	D	1134	0	1108	9	0
All	All	4536	0	4432	52	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 6.

The worst 5 of 52 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:74:PRO:HG2	1:C:79:LEU:HD11	1.66	0.78
1:D:74:PRO:HG2	1:D:79:LEU:HD11	1.68	0.76
1:B:74:PRO:HG2	1:B:79:LEU:HD11	1.74	0.70
1:B:60:ALA:HA	1:B:64:LEU:HD12	1.73	0.69
1:A:74:PRO:HG2	1:A:79:LEU:HD11	1.75	0.68

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	137/337 (41%)	132 (96%)	5 (4%)	0	100	100
1	B	137/337 (41%)	132 (96%)	5 (4%)	0	100	100
1	C	137/337 (41%)	134 (98%)	3 (2%)	0	100	100
1	D	137/337 (41%)	133 (97%)	4 (3%)	0	100	100
All	All	548/1348 (41%)	531 (97%)	17 (3%)	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	125/269 (46%)	125 (100%)	0	100	100
1	B	125/269 (46%)	125 (100%)	0	100	100
1	C	125/269 (46%)	125 (100%)	0	100	100
1	D	125/269 (46%)	125 (100%)	0	100	100
All	All	500/1076 (46%)	500 (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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

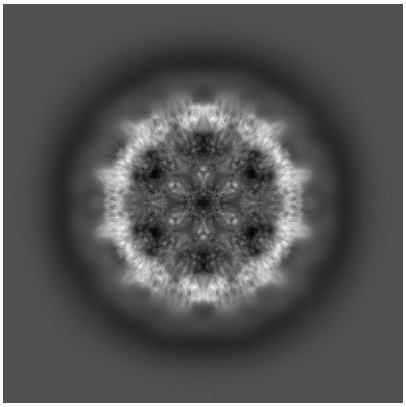
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31234. These allow visual inspection of the internal detail of the map and identification of artifacts.

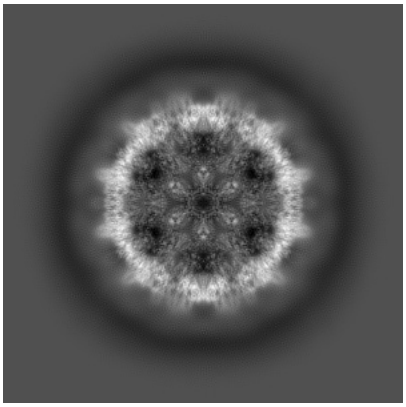
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

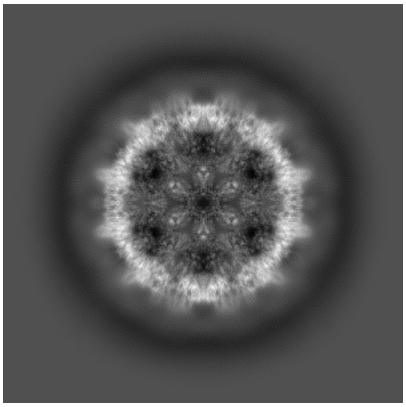
6.1.1 Primary map



X



Y

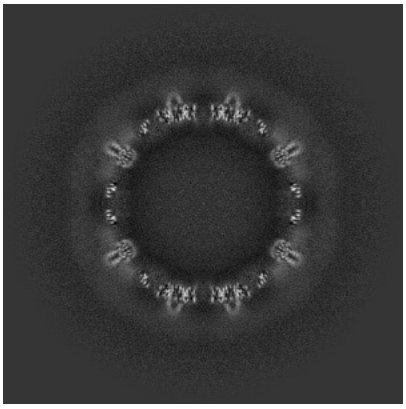


Z

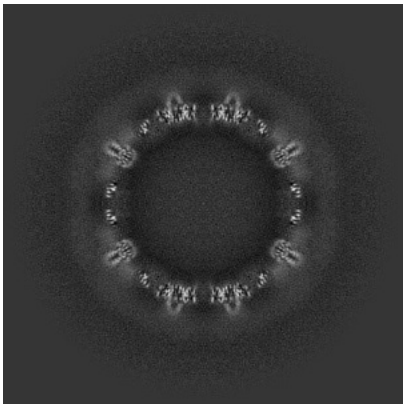
The images above show the map projected in three orthogonal directions.

6.2 Central slices

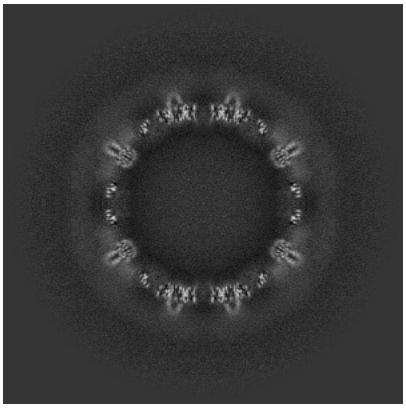
6.2.1 Primary map



X Index: 225



Y Index: 225

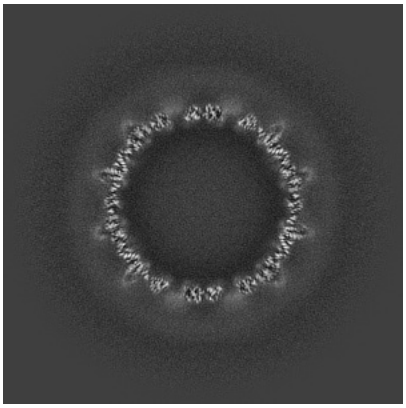


Z Index: 225

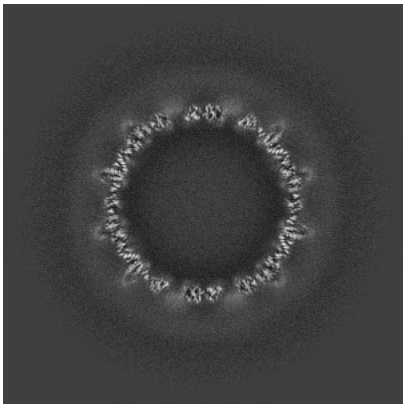
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

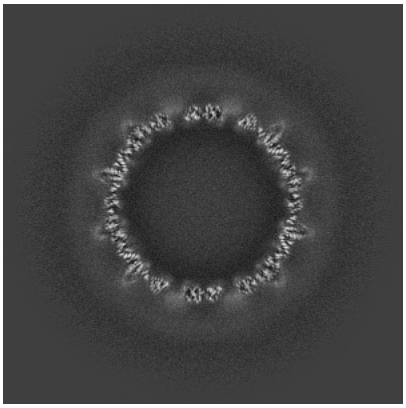
6.3.1 Primary map



X Index: 206



Y Index: 206

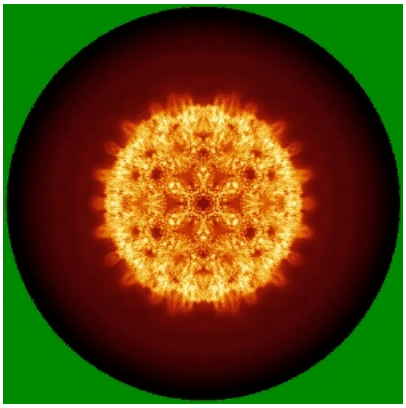


Z Index: 206

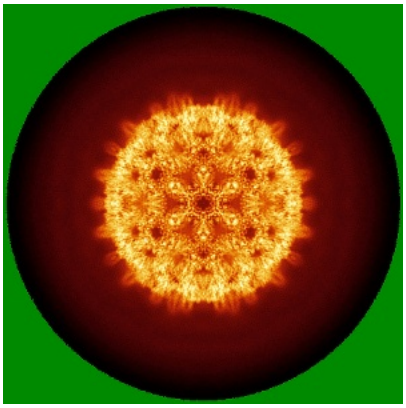
The images above show the largest variance slices of the map in three orthogonal directions.

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

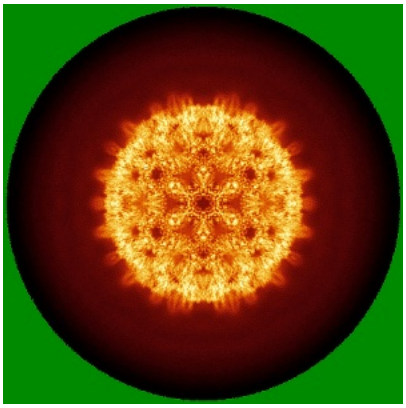
6.4.1 Primary map



X



Y

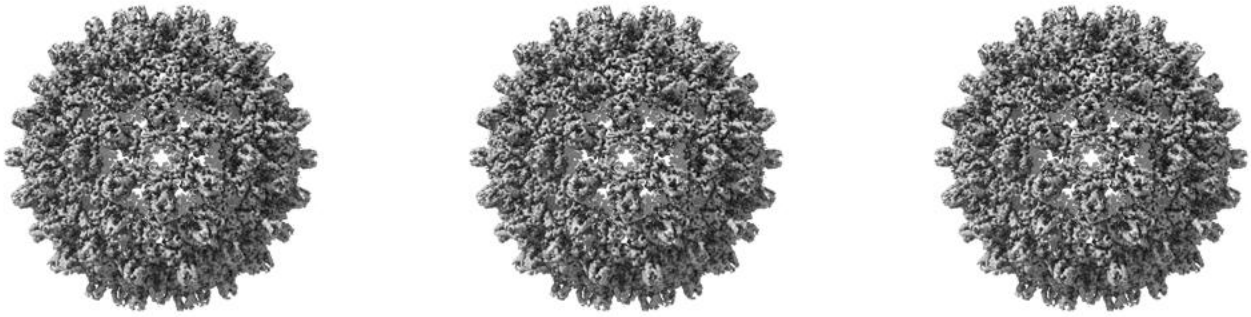


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.67. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

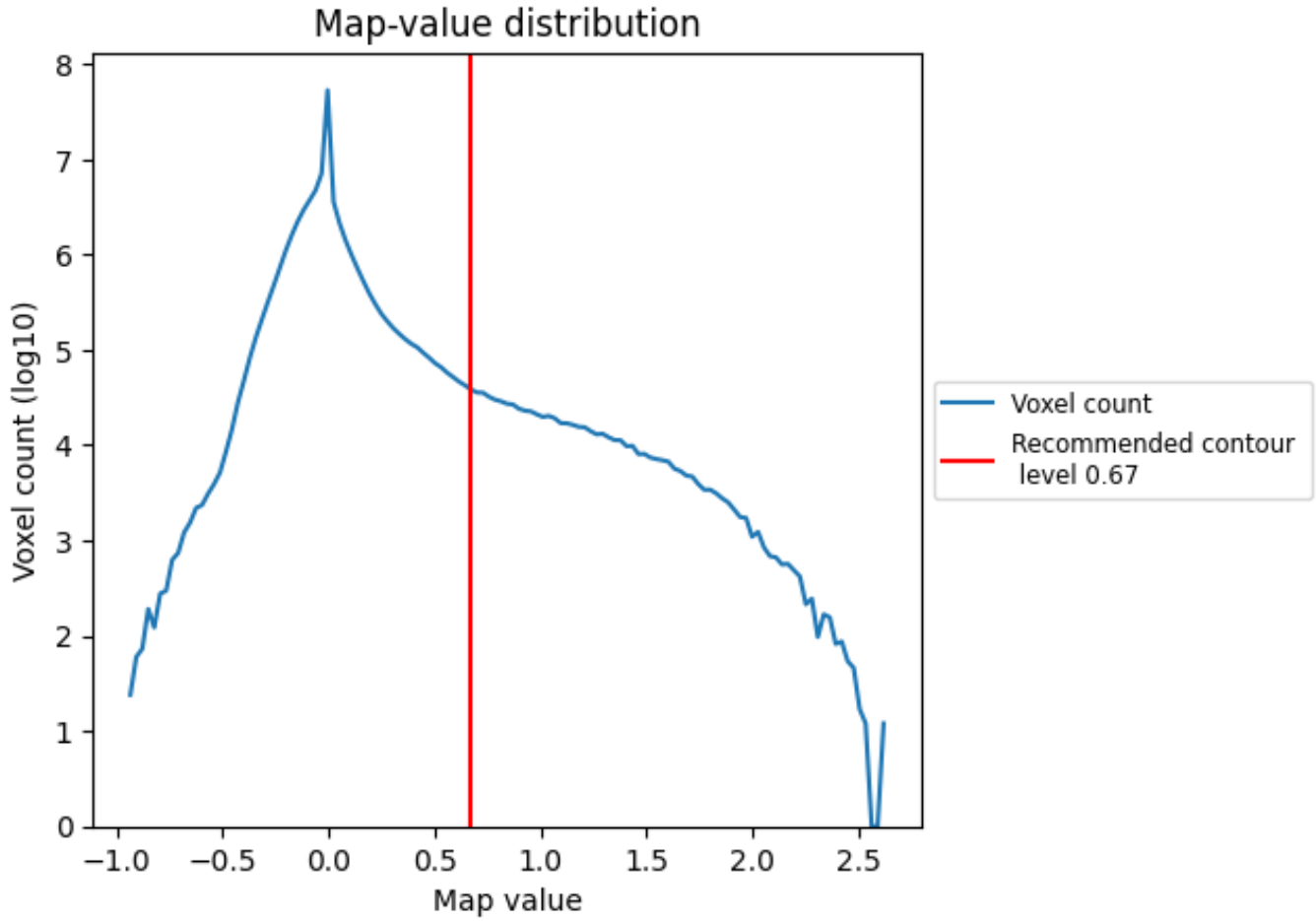
6.6 Mask visualisation (i)

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

7 Map analysis

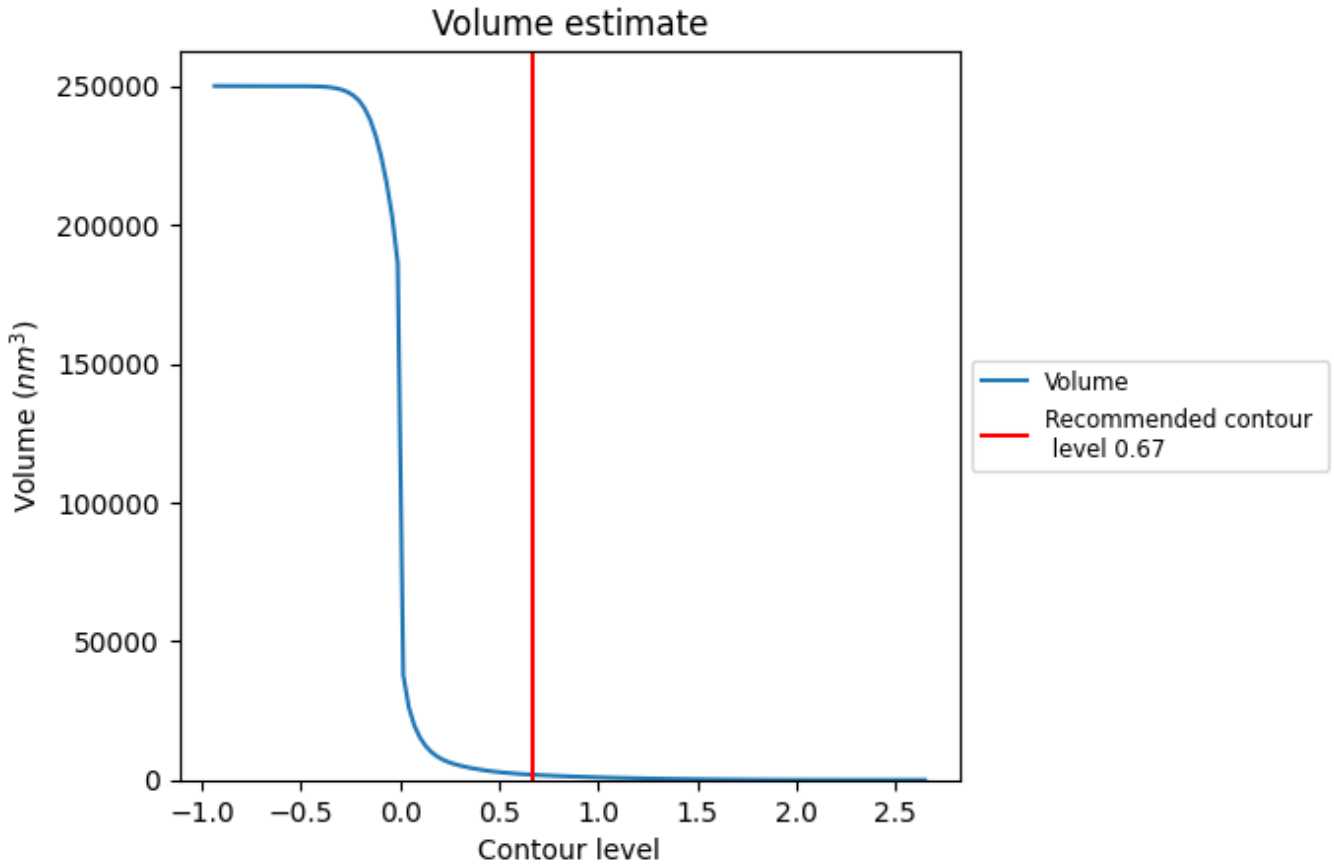
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

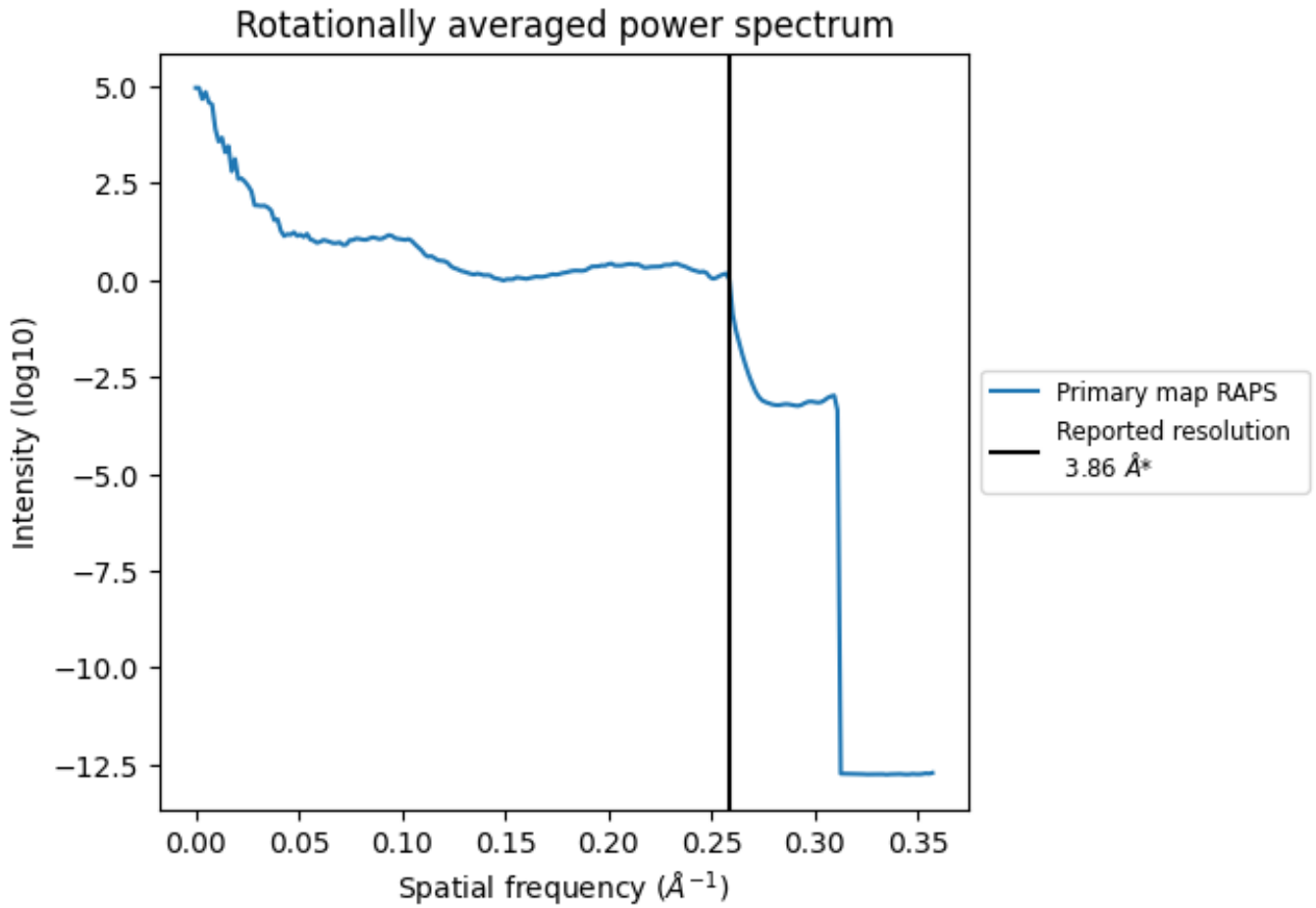
7.2 Volume estimate (i)



The volume at the recommended contour level is 1874 nm^3; this corresponds to an approximate mass of 1692 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 0.259 $Å^{-1}$

8 Fourier-Shell correlation

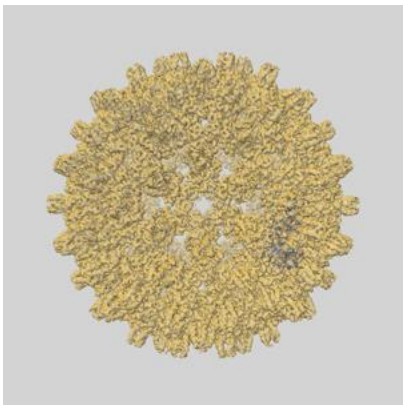
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

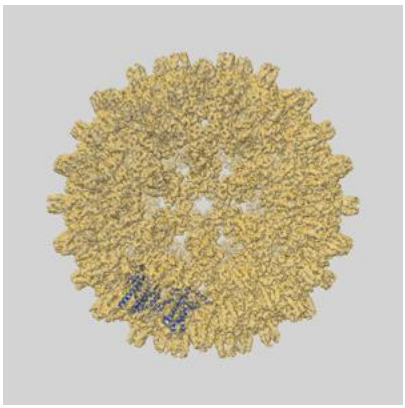
This section contains information regarding the fit between EMDB map EMD-31234 and PDB model 7EP6. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlays

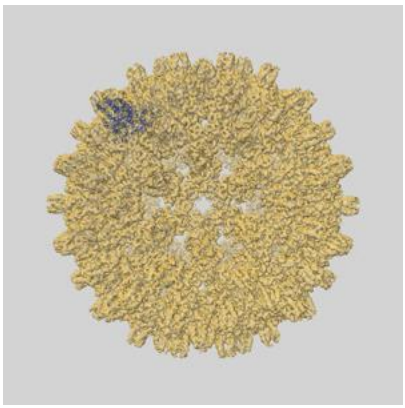
9.1.1 Map-model overlay



X

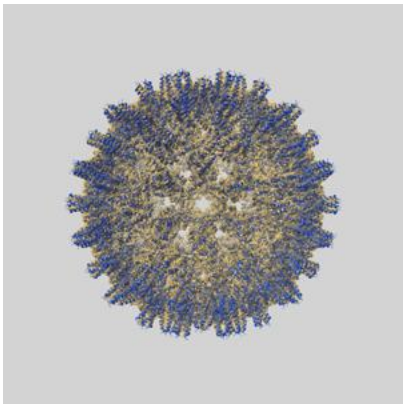


Y

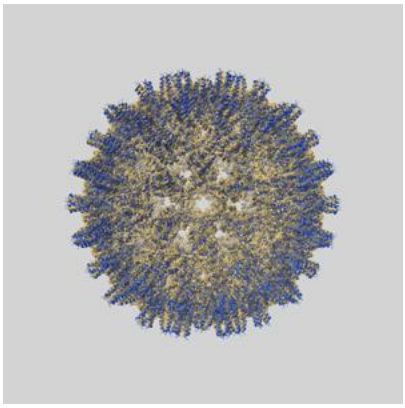


Z

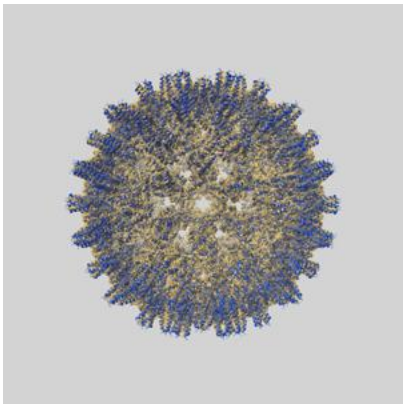
9.1.2 Map-model assembly overlay



X



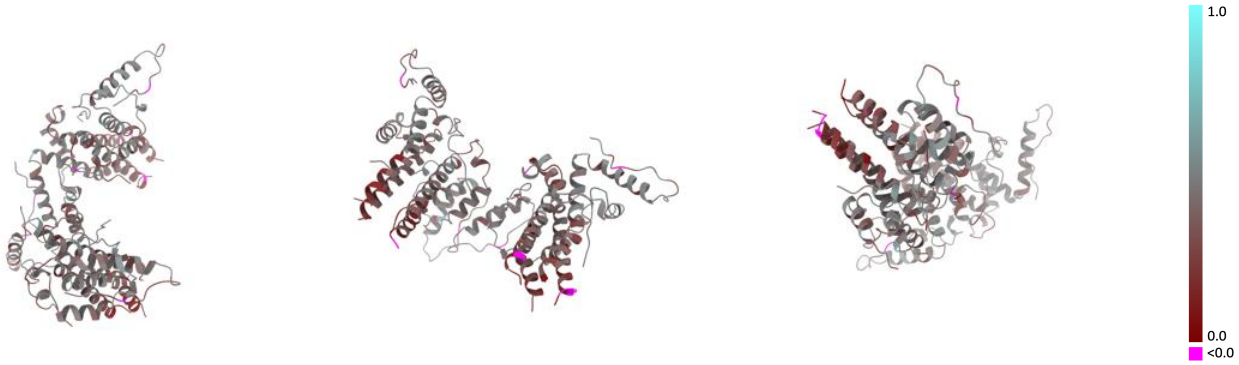
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.67 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.

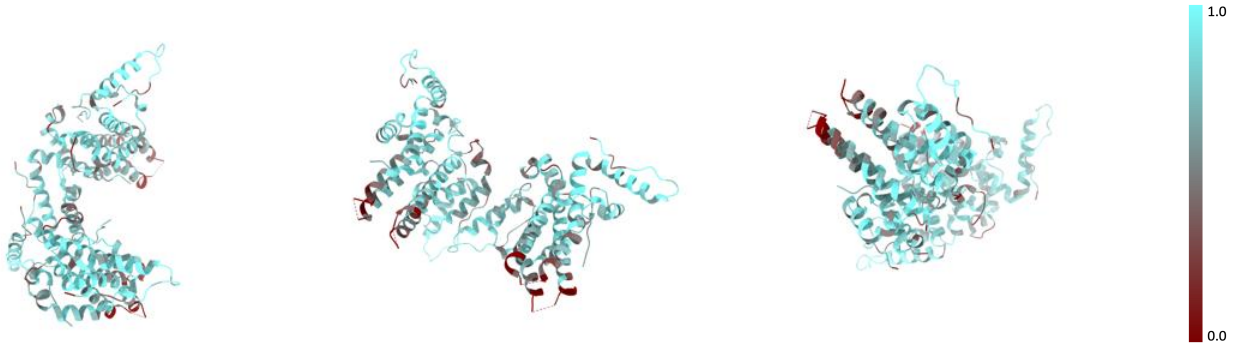
9.2 Q-score mapped to coordinate model



X Y Z

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.

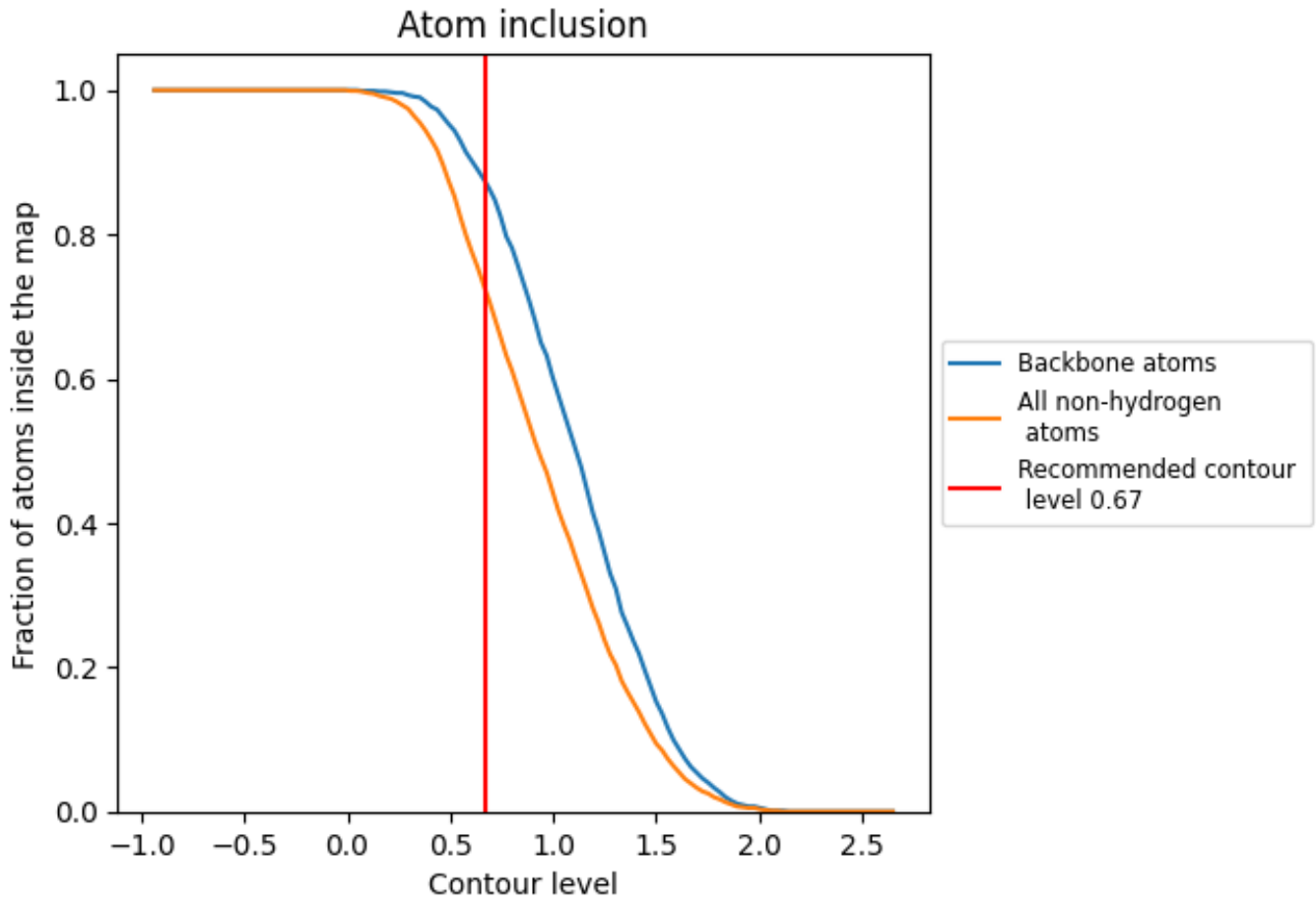
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.67).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.67) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.3970
A	0.7240	0.3900
B	0.7080	0.4040
C	0.7260	0.4020
D	0.7340	0.3940