W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 11, 2024 – 05:54 PM JST

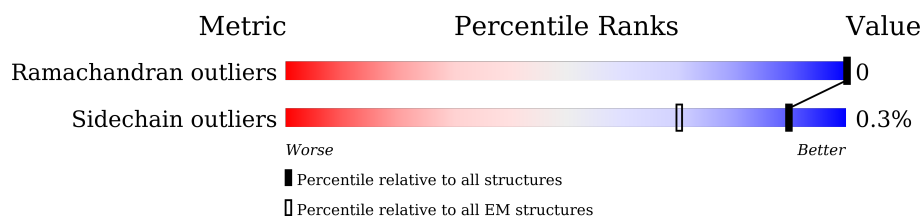|		
PDB ID	:	7ET3
EMDB ID	:	EMD-31297
Title	:	C5 portal vertex in the enveloped virion capsid
Authors	:	Li, Z.; Yu, X.
Deposited on	:	2021-05-12
Resolution	:	4.20 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
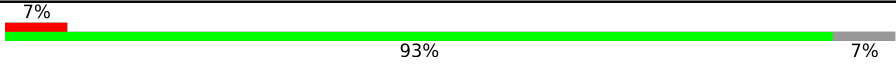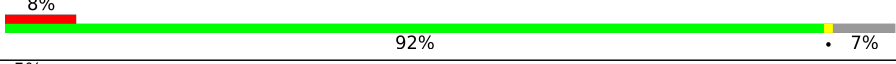*ELECTRON MICROSCOPY*
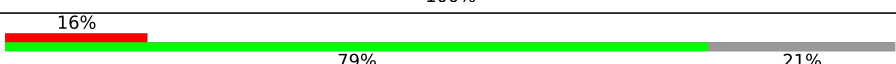
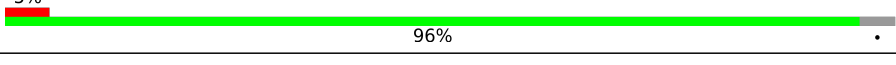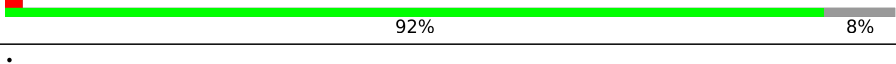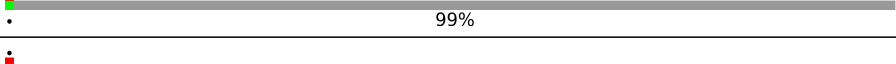The reported resolution of this entry is 4.20 Å.

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	Percentile Ranks	Value
Ramachandran outliers		0
Sidechain outliers		0.3%

Worse   *Better*

▌Percentile relative to all structures
▯Percentile relative to all EM structures
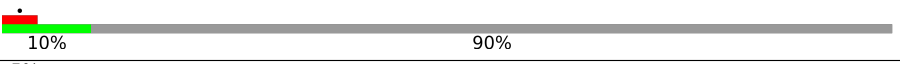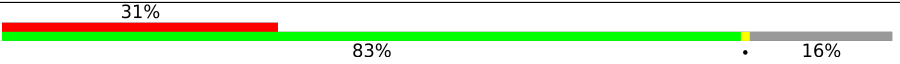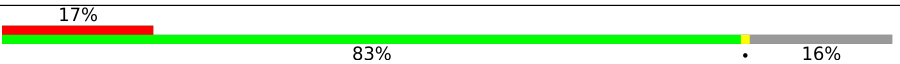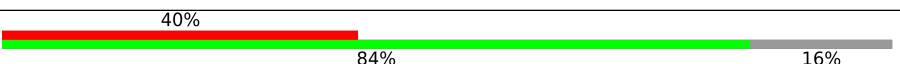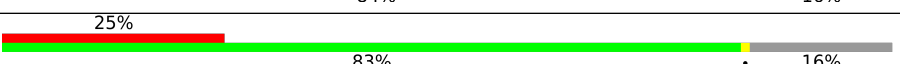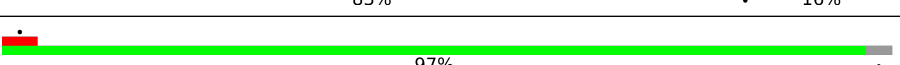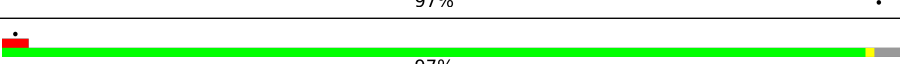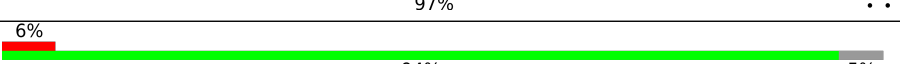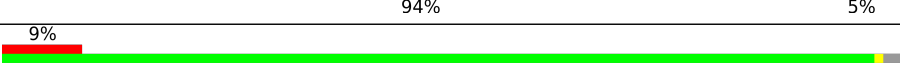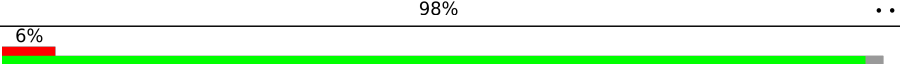
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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.

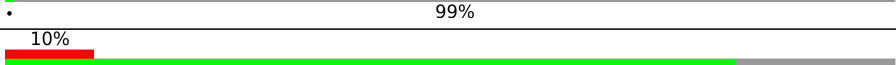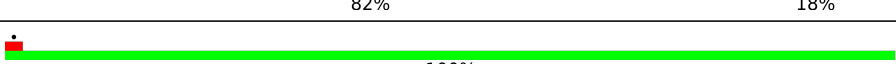| Mol	Chain	Length	Quality of chain
1	I	306	7% / 93% / 7%
1	h	306	8% / 92% / 7%
1	n	306	5% / 96% / •
1	o	306	• / 92% / 8%
2	H	2241	• / 99%
2	P	2241	• / 99%
3	g	290	10% / 82% / 18%
3	m	290	• / 100%
4	M	594	16% / 79% / 21%

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Mol	Chain	Length	Quality of chain
5	N	642	10% 90%
5	O	642	5% 11% 89%
6	1	1048	8% 27% 73%
7	R	75	31% 83% 16%
7	S	75	17% 83% 16%
7	T	75	57% 83% 16%
7	i	75	40% 84% 16%
7	j	75	25% 83% 16%
8	B	1370	97%
8	C	1370	97%
8	D	1370	6% 94% 5%
8	Y	1370	9% 98%
8	Z	1370	6% 97%
8	a	1370	94% 6%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 86332 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 Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	h	285	Total	C	N	O	S	0	0
			2258	1454	386	402	16		
1	I	285	Total	C	N	O	S	0	0
			2264	1454	389	404	17		
1	n	293	Total	C	N	O	S	0	0
			2322	1493	400	410	19		
1	o	282	Total	C	N	O	S	0	0
			2239	1442	382	397	18		

- Molecule 2 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	20	Total	C	N	O	S	0	0
			172	110	32	29	1		
2	P	20	Total	C	N	O	S	0	0
			172	110	32	29	1		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	237	Total	C	N	O	S	0	0
			1896	1218	332	335	11		
3	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	468	Total	C	N	O	S	0	0
			3848	2408	740	686	14		

- Molecule 5 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	65	Total 551	C 341	N 110	O 96	S 4	0	0
5	O	69	Total 589	C 371	N 113	O 102	S 3	0	0

- Molecule 6 is a protein called ORFL92C_UL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	285	Total 2328	C 1468	N 426	O 421	S 13	0	0

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	63	Total 513	C 321	N 97	O 91	S 4	0	0
7	S	63	Total 513	C 321	N 97	O 91	S 4	0	0
7	T	63	Total 513	C 321	N 97	O 91	S 4	0	0
7	i	63	Total 513	C 321	N 97	O 91	S 4	0	0
7	j	63	Total 513	C 321	N 97	O 91	S 4	0	0

- Molecule 8 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	1286	Total 10169	C 6469	N 1770	O 1871	S 59	0	0
8	B	1332	Total 10567	C 6728	N 1831	O 1947	S 61	0	0
8	C	1330	Total 10540	C 6713	N 1830	O 1936	S 61	0	0
8	D	1297	Total 10269	C 6538	N 1785	O 1887	S 59	0	0
8	Y	1347	Total 10676	C 6799	N 1850	O 1966	S 61	0	0
8	Z	1337	Total 10582	C 6740	N 1831	O 1952	S 59	0	0

3   Residue-property plots ⓘ

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: Triplex capsid protein 2
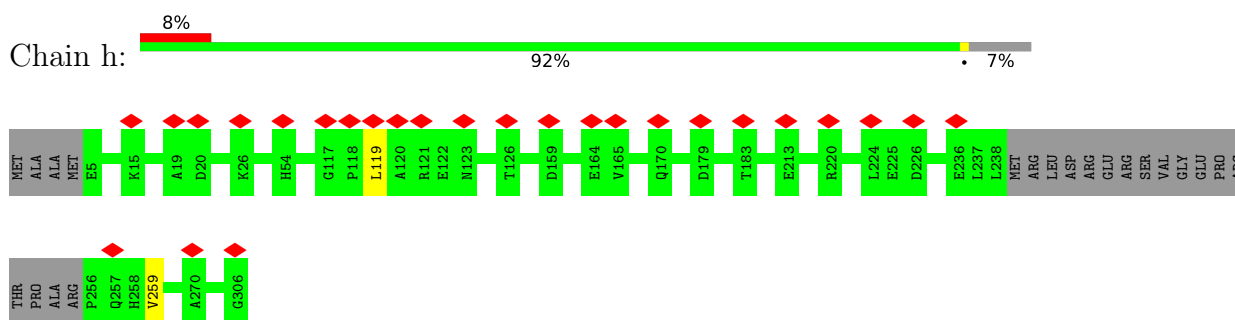
- Molecule 1: Triplex capsid protein 2
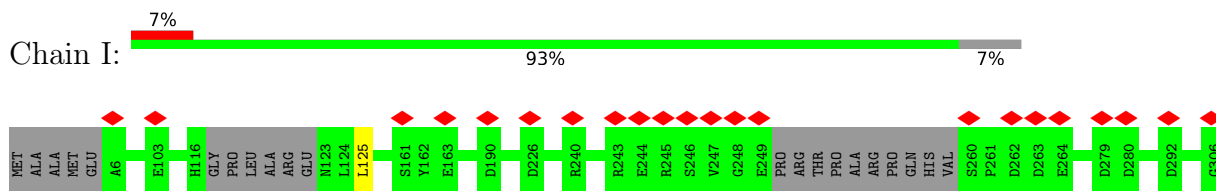
- Molecule 1: Triplex capsid protein 2
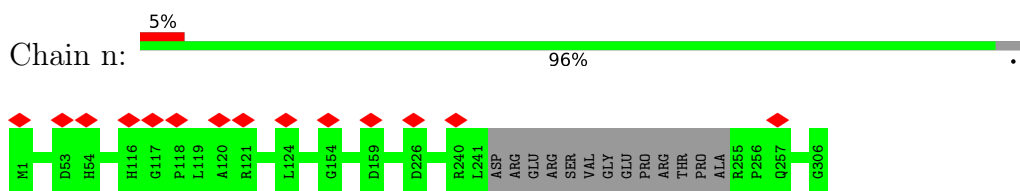
- Molecule 1: Triplex capsid protein 2

- Molecule 2: Large tegument protein deneddylase

MET LYS VAL THR GLN ALA SER CYS HIS GLN GLY ASP ILE ALA ARG PHE GLY ALA ARG ALA GLY ASN GLN CYS VAL CYS ASN GLY ILE MET PHE LEU HIS ALA LEU HIS LEU GLY THR SER ALA VAL LEU GLU THR GLU LEU ASP ALA ILE MET GLU GLY ALA ARG LEU ASP

ALA ARG LEU GLU ARG GLU LEU GLN LYS LYS LEU PRO ALA GLY GLY LEU PRO VAL TYR ARG LEU GLY ASP GLU VAL PRO ARG ARG LEU GLU LEU SER ARG PHE GLY ARG THR VAL HIS ALA LEU SER ARG PRO PHE ASN GLY THR GLU THR GLY THR CYS ASP ALA ASP GLY TYR MET CYS PRO

GLY ILE PHE PHE LEU TYR ALA ARG HIS ALA LYS ARG PRO THR TYR VAL VAL LEU THR VAL LEU ASN SER LEU ALA ARG ALA VAL VAL PHE GLU GLY ASP ASP HIS SER MET LEU VAL ASP PRO HIS SER SER ALA GLU GLY CYS HIS ALA ALA VAL TYR HIS CYS GLU LEU HIS GLN

VAL LEU MET LEU THR GLY PHE GLY VAL GLN LEU SER PRO ALA PHE TYR TYR GLU ALA LEU PHE LEU TYR MET LEU ASP VAL ALA THR VAL PHE GLU ASP ALA GLU ILE ALA ALA ARG VAL SER THR TYR ARG ASP ASP ILE ASP THR GLY VAL VAL ARG SER ALA ASP

THR ALA ALA THR THR THR ALA ALA PRO SER LEU PRO PRO LEU PRO ASP PRO ILE VAL ASP PRO GLY CYS PRO PRO GLY VAL VAL ALA PRO ILE ALA ALA SER ILE PRO VAL TYR ASP PRO SER SER PRO LYS LYS THR PRO GLU LYS ARG ARG LYS ASP SER LEU SER LYS HIS GLY GLY LYS

LYS LYS PRO SER THR THR THR SER SER LYS THR LEU ALA ALA THR ALA SER SER PRO SER ALA ILE ALA ALA SER SER SER ALA VAL PRO PRO SER SER CYS GLY GLY GLY ALA LEU PRO ALA LEU GLY ARG TYR ASP SER PRO SER SER PRO LYS LYS THR PRO ARG GLN LEU ASP GLU SER GLY SER LYS SER GLY LYS GLY VAL GLN LEU LYS LYS LEU ALA

LEU THR LEU PRO PRO LEU PRO ALA ASN THR SER ALA TRP THR LEU ALA HIS ALA ALA GLY THR GLU GLY SER GLY ALA ASN ALA ALA THR ALA THR ALA PRO SER PHE ASP GLU ALA PHE LEU THR ASP ARG LEU GLN LEU GLY LEU ILE ILE HIS ALA VAL ASN GLN SER CYS LEU ARG ARG PRO

CYS GLY PRO GLN ALA ALA GLN GLN ALA VAL ARG ALA TYR LEU GLY LEU SER LYS LEU ASP PHE LEU ASN TRP LEU HIS HIS GLY LEU ASP LEU ARG MET HIS ASP TYR LEU SER HIS THR THR GLY THR LYS ASP THR TYR SER THR LEU ASP ARG ALA LEU LEU GLU

LYS MET GLN VAL VAL PHE ASP PRO TYR GLY ARG GLN HIS GLY PRO ALA LEU ILE ALA TRP VAL GLU GLU MET LEU ARG TYR VAL SER GLY HIS VAL LEU TYR GLU HIS LEU GLY LEU ALA GLY LEU THR THR LYS ARG PRO MET PRO VAL SER ASP SER PHE VAL CYS LEU ARG PRO

VAL ASP PHE GLN LEU LEU THR GLN VAL ILE GLU GLN ARG ARG VAL LEU GLN ARG ARG GLU GLU TYR HIS GLY VAL TYR LEU GLU HIS GLY LEU ALA GLY LEU GLU THR SER ILE ILE HIS ASP LEU ASP SER ASP ASN ARG GLU ILE LEU LYS ALA LEU GLN PRO LEU

ASP ASP ASN ALA LYS GLN GLU LEU PHE ARG LEU GLY ASN ALA LYS MET LEU GLU GLU LEU GLN MET ASP LEU ASP ARG LEU SER THR GLU GLN LEU GLU LEU THR ARG VAL HIS ASN HIS ILE LEU ASN GLY PHE LEU PRO VAL GLU ASP LYS MET PRO ARG VAL GLU VAL GLN PRO LEU ARG

LEU PHE TYR ASP ARG ASP LYS LEU CYS ASP GLY SER TYR GLU GLY PHE VAL LEU ILE ARG GLU GLN GLN SER TYR LEU MET THR GLY THR VAL ASP HIS ASN HIS ILE LEU ASN GLY PHE LEU PRO VAL GLU ASP LYS HIS ALA TYR GLN ALA THR GLN GLN ASN GLU GLY

ARG LEU THR ILE HIS ASP LEU HIS VAL ILE GLU THR LEU VAL ARG ASP PRO GLY SER ARG GLY SER ALA LEU THR LEU ALA LEU VAL GLN GLN LEU ALA GLN GLU GLY ALA LEU GLY LEU GLN GLN GLU ARG HIS ALA TYR GLN ALA THR GLN GLN ASN ALA LEU GLU ALA LEU

SER ARG LEU GLU GLU GLU GLU GLU GLN GLN THR GLN ARG PHE LEU ASP LEU GLY LEU SER ASP ASP PRO ASN GLU GLN THR ILE LYS ARG HIS PRO GLN LEU ARG GLU GLU MET ALA ARG ARG ASP GLU GLN GLN THR ARG LEU ARG ILE ASN ALA VAL LEU SER MET PHE HIS THR LEU VAL

MET ARG LEU ALA ARG ASP GLU SER PRO ARG PRO THR PHE PHE ASP ALA VAL SER LEU LEU GLN LEU PRO ASP SER HIS GLU GLU ASP GLU LEU ARG ALA ALA ASN ALA THR TYR ALA GLN MET VAL LYS LYS LEU GLU GLN ILE GLU GLU LYS GLY THR ALA SER GLU

LYS ARG PHE GLN ALA LEU ARG GLU GLU LEU VAL TYR PHE PHE ARG ASN HIS GLU TYR PHE PHE GLN HIS MET VAL GLY ARG LEU ILE GLY VAL GLY PRO GLN LEU THR LEU GLU THR LYS MET GLU HIS GLU GLU GLN GLN HIS LEU GLU GLU ARG GLU ARG GLU ARG GLU TRP GLU GLU ALA

GLY LYS LEU THR VAL THR SER VAL GLU ASP VAL GLN VAL LYS ARG VAL LEU ALA ARG ALA PRO SER HIS ARG VAL MET HIS GLN MET GLN GLN THR LEU THR LEU THR LYS MET GLN ASP PHE ASP GLU LYS GLU TYR GLN HIS GLU MET GLU GLN GLN HIS LEU GLU GLU LEU ASP GLY TYR GLN LYS LYS

VAL GLN GLN ASP GLN LEU GLN ARG VAL ASP ALA VAL LYS LEU ARG GLY ASP MET LEU SER THR ILE PRO SER HIS ARG VAL MET GLN GLN MET GLN GLN THR LEU LEU LEU GLY LEU ASP ARG ALA LEU LEU GLN GLN GLN LEU ASP SER ALA LEU GLN GLN GLN LEU GLN SER LYS LYS

LEU ASP GLY ARG ILE ASN GLU GLU CYS LEU HIS GLY VAL LEU THR GLY ASP VAL GLU ARG CYS HIS PRO GLN HIS ARG GLN LEU GLU ALA ALA MET GLN THR GLN ALA SER LEU ASN HIS GLU ASP ILE LEU GLY PRO GLN ALA LEU GLU LEU ILE HIS GLU THR GLN GLN LEU GLN ASN GLU GLU GLY

GLN ALA GLN PHE ILE GLU LYS CYS GLN GLN GLY ASP PRO THR THR ALA ILE THR GLY SER GLU SER GLU GLN LYS MET GLU GLN LEU GLU GLN GLU GLY TYR ARG SER GLU SER ALA LEU GLN LEU GLN LEU GLN HIS ALA VAL HIS THR SER GLU THR GLU THR SER GLU ARG LEU ASP ARG ARG SER LEU ARG GLN

Row 1: ASP PRO GLY SER SER VAL THR ARG VAL PRO GLU LYS PRO PHE LYS GLY GLN LEU ALA GLY ARG ILE THR PRO PRO ALA ASP PHE GLN PRO VAL PHE LYS THR LEU ASP GLN GLN ALA ALA ARG LYS ALA LEU SER ASP GLN ALA ASP LEU LEU ASN GLN

Row 2: LYS VAL GLN THR GLN LEU ARG GLN ARG ASP GLU GLN LEU SER THR ALA GLN ASN LEU TRP THR ALA GLN LEU VAL THR ARG HIS LYS MET SER GLY LEU ASP VAL THR THR PRO ASP ALA LYS ALA LEU MET GLU LYS PRO LEU GLU THR ARG GLU LEU GLY ALA THR GLN

Row 3: GLN LEU PRO TYR LEU SER GLU ARG ALA THR VAL ARG MET LEU ALA LEU GLU GLU ALA LEU LEU ALA GLN ILE THR ALA ASP PRO THR HIS PRO HIS HIS GLY SER ARG ARG HIS TYR ARG ASN LEU GLN GLN ALA VAL GLU VAL SER ALA VAL THR ALA HIS ILE GLU GLN

Row 4: ASN ALA ALA CYS GLU ASN PHE ILE ALA GLN HIS GLN ALA GLU THR ALA ASN GLY SER ALA THR PRO ARG VAL ASP MET VAL GLN ALA VAL GLU ALA TRP GLN ARG LEU GLU PRO GLY ARG VAL GLY ALA ALA ARG HIS GLN LYS VAL GLN LEU LEU GLN ARG LEU GLY

Row 5: GLN THR LEU GLY ASP LEU GLU LEU GLN GLU THR LEU ALA THR LEU GLU TYR PHE ALA LEU LEU HIS GLY ILE GLN THR PHE SER TYR GLY LEU ASP PHE ARG SER GLN LEU GLU LEU LYS ILE ARG ASP LEU THR ARG ALA PHE ALA LEU ALA LYS ARG ARG GLY THR ARG SER ASN GLU

Row 6: GLY VAL LEU PRO ASN PRO ARG LYS PRO GLN ALA THR SER LEU GLY ALA PHE THR ARG GLY LEU ASN ALA LEU GLU ARG HIS VAL GLN LEU GLY HIS GLN TYR LEU LEU ASN LYS LEU ASN GLY SER SER VAL TYR ARG GLU ASP ILE PRO SER VAL LEU PRO ALA THR HIS

Row 7: GLU THR ASP ALA LEU ILE MET ARG ARG LEU ARG LEU CYS PHE ALA ARG HIS HIS ASP THR PHE LEU GLU VAL VAL ASP VAL PHE GLY MET ARG GLN ILE VAL THR GLN ALA GLY GLU ILE HIS LEU VAL THR ASP TYR GLY ASN VAL ALA PHE LYS TYR LEU ALA LEU

Row 8: ARG ASP ASP GLY ARG PRO LEU ALA TRP ARG ARG ARG CYS SER GLY GLY LEU LYS ASN VAL THR THR ARG TYR LYS ALA ILE GLU THR VAL ALA VAL CYS GLN THR LEU ARG THR PHE TRP PRO GLN ILE SER GLN TYR ASP LEU ARG PRO TYR LEU THR GLN HIS GLN SER

Row 9: HIS THR HIS PRO ALA GLU THR HIS THR LEU HIS ASN LEU LYS LEU LEU PHE CYS TYR LEU VAL SER THR ALA TRP GLN ARG ILE ASP THR GLN GLN LEU THR ALA HIS LEU GLN ASP VAL GLY SER GLY GLU GLY GLY ASP VAL GLY GLN GLN ARG PRO ARG GLY THR VAL LEU ARG

Row 10: LEU SER LEU GLN PHE CYS VAL LEU ILE ALA ALA LEU TYR PRO GLU TYR ILE TYR THR VAL LEU LYS TYR PRO VAL GLN MET SER LEU PRO SER LEU THR ALA HIS LEU HIS GLN ASP VAL ILE HIS ALA VAL VAL ASN THR HIS LYS MET PRO PRO ASP HIS LEU PRO GLU GLN

Row 11: VAL LYS ALA PHE CYS ILE THR THR PRO THR GLN TRP PRO ALA MET GLN LEU ASN LYS LEU PHE TRP GLU ASN LYS LEU VAL GLN GLN LEU CYS GLN VAL GLY PRO GLN LYS SER THR PRO LEU GLY LYS LEU TRP LEU TYR ALA MET ALA THR LEU VAL PHE PRO GLN ASP MET LEU GLN

Row 12: CYS LEU TRP LEU GLU LEU LYS PRO GLN TYR ALA GLU GLY THR ALA SER VAL SER GLU LEU VAL GLN LEU PHE GLN ILE PHE THR GLN GLN CYS GLN VAL GLY MET VAL THR GLU GLY TYR THR GLN PRO GLN LEU LEU PRO THR GLY GLU PRO VAL LEU GLN MET ILE ARG GLN ASP

Row 13: THR THR THR ASP THR ASN THR THR GLU PRO GLY LEU LEU ASP ASP VAL PHE ILE GLN GLU THR ALA LEU ASP TYR ALA LEU GLY SER TRP LEU GLY ILE PRO VAL CYS LEU GLY VAL HIS VAL ALA ASP LEU LYS GLY GLN ARG ILE LEU VAL ALA ARG HIS LEU GLU

Row 14: TYR THR SER ARG ASP ARG PHE ASP LEU ARG ILE GLN GLN ARG SER ARG LEU ASN LEU GLN LEU GLN ASP THR TRP THR GLU ASP THR LEU PRO GLN GLU HIS CYS TRP LEU GLN ALA GLN ILE ARG LEU ARG ASP TYR ARG ARG PHE LEU THR ARG ILE GLU PHE ILE PRO LEU VAL

Row 15: ILE TYR ASN ALA GLN ASP HIS THR VAL VAL ARG VAL ARG PRO SER THR PHE GLU GLN ASP HIS SER ARG VAL LEU LEU ASP GLU PHE PRO PHE LEU TYR ASP GLN ASP ASN SER ALA ASP ILE ALA SER GLY ALA ALA PRO THR PRO PRO VAL

Row 16: PRO PHE ASN ARG VAL PRO VAL ASN ILE PHE LEU ARG GLU ASN PRO PRO ILE ALA ARG VAL GLN PRO PRO ARG ARG HIS ARG HIS ARG ALA ALA ALA ASP ASP GLY GLN ILE ASP HIS VAL GLN LEU ASP ASP THR SER ARG THR ALA ASP SER ALA LEU VAL SER

Row 17: THR ALA PHE GLY SER VAL PHE GLN GLU ASN ARG LEU GLY GLU ASN THR PRO LEU CYS ARG ASP GLU LEU VAL ALA VAL ALA PRO GLY ALA ALA SER THR SER PHE ALA SER PRO PRO ILE THR VAL LEU THR GLN ASN VAL LEU SER ALA LEU GLU ILE LEU ILE LEU ARG LEU VAL ARG LEU ASP

● Molecule 2: Large tegument protein deneddylase

Chain P: 99%

MET LYS VAL THR GLN ALA SER CYS HIS GLN GLY ASP ILE ALA ARG PHE GLY ALA ARG ALA GLY ASN GLN CYS VAL CYS ASN GLY ILE MET PHE LEU HIS ALA LEU HIS LEU GLY GLY THR SER ALA VAL LEU GLN THR GLU ALA LEU ASP ALA ILE MET GLU GLY ALA ARG LEU ASP

ALA ARG LEU GLU ARG GLU GLU LEU LYS LYS LEU PRO ALA GLY GLY ARG LEU PRO VAL TYR ARG LEU GLY ASP GLU VAL PRO ARG ARG LEU GLU GLY SER PHE GLY ARG THR VAL HIS ALA LEU SER ARG PRO PHE ASN GLY THR GLU THR THR CYS ASP ASP GLY TYR MET CYS PRO

GLY ILE PHE ASP PHE LEU TYR ALA ARG TYR ALA HIS ALA LYS ARG PRO THR TYR VAL LEU VAL LEU THR VAL ASN SER LEU ALA ARG ALA VAL PHE GLU THR GLU ASP HIS MET LEU VAL ASP PRO HIS SER SER ALA GLU GLU CYS HIS ASN ALA ALA VAL TYR HIS CYS GLU GLY LEU HIS GLN

VAL LEU MET LEU THR GLY PHE GLY VAL GLN LEU PRO ALA SER PRO ALA PHE TYR TYR GLU ALA LEU PHE LEU TYR MET LEU ASP VAL ALA THR VAL PHE GLU GLU ILE ALA ALA ARG VAL SER THR TYR ARG ASP ARG ASP ILE ASP LEU ASP THR GLY VAL VAL ARG SER ALA ASP

THR ALA ALA THR THR THR THR ALA ALA PRO SER LEU ASP PRO LEU PRO ASP PRO ILE VAL ASP PRO GLY CYS PRO GLY VAL ALA PRO ILE ALA ALA SER SER SER ALA VAL PRO PRO SER SER CYS GLY GLU GLY TYR ASP PRO SER SER PRO LYS LYS THR PRO GLU ARG ARG LYS ASP SER GLY LYS LYS

LYS LYS PRO SER THR THR THR SER LYS THR LEU ALA THR ALA SER SER PRO SER ALA ILE ALA ALA SER SER SER ALA VAL PRO PRO SER SER CYS GLY GLU GLY TYR ALA LEU GLY ARG TYR GLN LEU ASP GLU VAL GLU GLN LEU ASP SER LYS HIS GLY GLY LYS

LEU THR LEU PRO LEU PRO LEU PRO ALA ASN THR SER ALA TRP THR LEU ALA HIS ALA ALA GLY THR GLU SER GLY ALA ASN ALA THR ALA THR ALA PRO SER PHE ASP GLU ALA PHE LEU THR ASP LEU GLN LEU ILE HIS ALA VAL ASN GLN SER CYS LEU ARG ARG PRO

CYS GLY PRO GLN SER ALA ALA GLN GLN ALA VAL ARG ALA TYR LEU GLY LEU SER LYS LEU ASP ALA PHE LEU ASN TRP LEU HIS HIS GLY LEU ASP GLU LEU GLN ARG MET HIS ASP TYR LEU SER HIS LYS THR THR LYS GLY THR LYS TYR SER THR THR LYS ASP ARG ALA LEU LEU GLU

LYS MET GLN VAL VAL PHE ASP PRO TYR GLY ARG GLN HIS GLY PRO ALA LEU LEU ILE ALA TRP VAL GLU GLU MET ARG TYR VAL GLU HIS LEU ALA GLY LEU THR ASN GLU GLU ILE THR SER ILE HIS ASP LEU ASP SER ASP LEU ASN ARG ARG GLU ILE LEU LYS ALA LEU GLN PRO LEU

VAL ASP PHE GLN ARG LEU THR GLN VAL ILE GLU GLN ARG ARG ARG VAL LEU GLN ARG GLN GLY GLU GLU TYR HIS GLY VAL TYR VAL GLU HIS LEU ALA GLY LEU GLU ILE THR SER ILE LEU ASP ALA SER ASP LEU ASN ARG ARG GLU ILE LEU LYS ALA LEU GLN PRO LEU

ASP ASP ASN ALA LYS GLN GLU LEU PHE ARG LEU GLY ASN ALA LYS MET LEU GLU LEU GLN LEU MET ASP LEU ASP ARG LEU SER THR GLN LEU GLU LEU THR ARG VAL HIS ASN HIS ILE LEU ASN GLY PHE LEU PRO VAL GLU ASP LEU LYS MET GLU ARG VAL GLU VAL GLN GLN VAL LEU ARG

LEU PHE TYR ASP LEU ARG ASP LYS LEU CYS ASP GLY SER TYR GLU GLU GLY PHE VAL VAL ILE ARG GLU GLN GLN SER TYR LEU MET THR GLY THR VAL ARG ASP ASP ASN HIS ILE LEU LEU GLN LEU GLU ARG HIS ALA TYR GLN ALA THR GLN GLN ASN GLU GLY GLY

ARG LEU THR GLN ILE HIS ASP LEU LEU HIS VAL ILE GLU LEU THR LEU VAL ARG ASP PRO GLY SER GLY SER ALA LEU THR LEU ALA LEU VAL GLN GLN LEU ALA GLN LEU GLU ALA LEU GLY GLY GLN LEU GLN LEU PRO GLU GLN VAL GLN ARG LEU GLN ASN ALA LEU GLU ALA LEU

SER ARG LEU GLU GLU GLU GLU GLN THR GLN ARG PHE LEU ASP GLY LEU SER ASP PRO ASN GLU GLN THR ILE LYS ARG HIS PRO GLN LEU ARG GLU GLU MET ARG ARG ASP GLU GLN THR ARG LEU ARG LEU ILE ASN ALA VAL LEU SER MET PHE HIS THR LEU VAL

MET ARG LEU ALA ASP ASP GLU SER PRO ARG PRO THR PHE PHE ASP ALA VAL SER LEU LEU LEU GLN LEU PRO ASP SER HIS GLU GLU ASP LEU ARG ALA ALA ASN ALA THR TYR ALA MET VAL LYS LYS LEU GLU ILE LEU GLY LYS LEU GLY THR ARG LEU ALA SER GLU

LYS ARG PHE GLN ALA LEU ARG GLU GLU LEU VAL TYR PHE PHE ARG ASN HIS GLU GLY TYR PHE PHE GLN HIS MET GLY VAL ARG LEU GLY ARG LEU VAL GLY VAL PRO GLN LEU VAL THR GLU LEU GLU TYR GLU GLN HIS GLU MET GLU GLN GLN HIS GLU ARG GLU LEU GLU GLU ALA

GLY LYS LEU THR VAL THR SER VAL GLU ASP VAL GLN VAL LEU ARG VAL LEU ALA ARG ALA PRO SER HIS ARG VAL MET HIS GLN MET GLN GLN THR LEU THR LEU THR LYS MET GLN ASP PHE ASP GLU LYS ARG LYS GLN GLU GLU GLN GLN GLN ARG LEU GLU ASP TRP THR GLY TYR LYS LYS

VAL GLN GLN ASP LEU GLN ARG VAL VAL ASP ALA VAL LYS LEU ARG THR GLY ASP MET LEU SER THR ILE PRO SER HIS ARG VAL MET GLN GLN THR LEU THR LEU LEU LYS MET GLN ASP PHE ASN GLN ASP LEU LEU SER ALA LEU GLN GLN GLN SER LYS LYS

LEU ASP GLY ARG ILE ASN GLU CYS LEU HIS GLY VAL LEU THR GLY ASP VAL GLU ARG CYS HIS PRO HIS ARG GLU ALA ALA MET LEU THR GLN ALA THR GLN LEU SER LEU ASN HIS GLU ASP GLN GLN ARG ALA LEU LEU ASP GLY TYR THR GLN LYS LYS

GLN ALA GLN PHE ILE GLU LYS GLN GLY GLY ASP PRO THR THR ALA ILE THR GLY MET GLY SER GLU SER GLN LYS MET GLN GLN LYS ASP PHE ALA ASP GLN PRO LEU LEU GLY GLN GLN LEU ILE HIS GLU THR GLN GLN MET THR GLU THR SER GLU ARG LEU ASP ARG SER LEU ARG GLN

ASP PRO GLY SER SER VAL THR ARG VAL PRO GLU LYS PRO PHE LYS GLY GLN LEU GLU GLU ALA GLY ARG ILE THR PRO PRO ALA ASP PHE GLN GLU PRO VAL PHE LYS THR LEU LEU ASP GLN GLN ALA ALA ARG LYS ALA LEU SER ASP GLU ALA ASP LEU LEU LEU ASN GLN

LYS VAL GLN THR GLN LEU ARG GLN ARG ASP GLU GLN LEU SER THR ALA GLN ASN LEU TRP THR LEU VAL THR ARG HIS LYS MET SER GLY GLY LEU ASP VAL THR PRO ASP ALA LYS ALA LEU MET GLU LYS PRO GLU LEU GLN THR LEU ARG GLU GLU LEU GLY LYS ALA THR GLN

GLN LEU PRO TYR LEU SER GLU ARG ALA GLU THR VAL ARG MET LEU ALA PHE LEU GLU GLU ALA LEU LEU ALA GLN ILE THR THR ALA ASP PRO THR HIS PRO HIS HIS GLY SER ARG ARG THR HIS TYR ARG ASN LEU GLN GLN GLN ALA VAL GLU SER ALA VAL THR LEU ALA HIS ILE GLU GLN

ASN ALA ALA CYS GLU ASN PHE ILE ALA GLN HIS GLN GLU ALA THR ALA ASN GLY SER ALA SER THR PRO ARG VAL ASP MET VAL GLN ALA VAL GLU ALA ALA TRP GLN ARG ARG LEU GLU PRO GLY ARG VAL ALA GLY GLN ALA ALA ARG HIS GLN LYS VAL GLN LEU LEU LEU ARG LEU GLY

GLN THR LEU GLY ASP LEU GLU GLU LEU GLN GLU THR LEU ALA THR LEU SER GLU TYR PHE ALA LEU LEU HIS GLY ILE GLN THR PHE SER TYR GLY LEU ASP PHE ARG SER GLN LEU GLU GLU LYS ILE ARG ASP LEU ARG THR ARG PHE ALA GLU LEU ALA LYS ARG ARG GLY THR ARG SER ASN GLU

GLY VAL LEU PRO ASN PRO ARG ARG LYS PRO GLN GLN ALA THR THR SER LEU GLY LEU ALA PHE LEU ARG GLY LEU ASN ALA LEU GLU GLN ARG HIS VAL GLN LEU GLY LEU HIS GLN TYR LEU LEU ASN LEU LEU ASN LYS GLN ASN ASP GLY SER SER LEU VAL TYR ARG LEU GLU ASP ILE PRO SER VAL LEU PRO ALA THR HIS

GLU THR ASP ALA LEU LEU ILE MET ARG ASP ARG LEU ARG ARG LEU CYS PHE ALA ARG HIS HIS ASP THR PHE LEU GLU VAL VAL ASP VAL GLN PHE GLY MET ARG GLN ILE VAL THR GLN ALA GLY GLU PRO ILE HIS LEU VAL ASP TYR GLY ASN VAL ALA PHE LYS TYR LEU ALA LEU

ARG ASP ASP GLY ARG PRO LEU ALA TRP ARG ARG ARG CYS SER GLY GLY LEU LYS ASN VAL THR VAL THR ARG TYR LYS ALA ILE THR VAL ALA VAL VAL CYS GLN THR LEU ARG THR PHE TRP PRO GLN ILE SER GLN GLN TYR ASP LEU ARG PRO TYR LEU THR GLN HIS GLN SER

HIS THR HIS PRO ALA GLU THR HIS HIS THR LEU HIS ASN LEU LYS LEU PHE CYS TYR LEU VAL SER THR ALA TRP GLN ARG ILE ASP THR GLN GLN LEU THR HIS ALA ASP VAL GLY SER GLY GLU GLY ASP VAL GLY LEU GLU GLN ARG PRO GLY ARG GLY THR VAL LEU ARG

LEU SER LEU GLN LEU PHE CYS VAL LEU ILE ALA ALA LEU TYR PRO GLU GLY TYR ILE TYR THR VAL LEU LEU TYR PRO VAL GLN MET SER LEU PRO SER LEU THR ALA HIS LEU GLN ASP VAL ILE HIS ALA VAL VAL ASN ASN THR HIS LYS MET PRO PRO ASP HIS LEU PRO GLU GLN

VAL LYS ALA PHE CYS ILE THR PRO THR GLN TRP PRO ALA MET GLN LEU ASN LYS LEU PHE TRP GLU LEU VAL GLN GLN LEU CYS GLN VAL GLY PRO GLN LYS SER THR PRO PRO LEU GLY LYS LEU TRP LEU ALA MET THR LEU VAL PHE PRO GLN ASP HIS LEU PRO GLU GLN

CYS LEU TRP LEU GLU LEU LYS PRO GLN TYR ALA GLU THR TYR ALA SER VAL LEU SER GLU LEU VAL GLN THR LEU PHE GLN ILE PHE THR GLN GLN CYS GLN VAL GLY MET VAL THR GLU GLY GLY TYR THR GLN PRO GLN LEU PRO THR GLY GLU PRO VAL LEU LEU GLN MET ILE ARG GLN ASP

THR THR THR ASP THR THR ASN THR THR THR GLU PRO GLY LEU LEU ASP SER VAL PHE ILE GLN LEU GLU THR ALA LEU ASP ASP TYR ALA LEU GLY SER GLU TRP LEU PRO GLY PHE ILE PRO VAL CYS LEU GLY VAL HIS VAL ALA ASP LEU LEU LYS GLY ARG ILE LEU VAL ALA ARG HIS LEU GLU

TYR THR SER ARG ASP ARG ASP PHE LEU ARG ILE GLN ARG SER ARG LEU ASN LEU SER GLN LEU GLN ASP THR TRP THR GLU THR PRO GLN GLU GLN HIS CYS TRP LEU GLN ALA GLN ILE GLU ARG LEU ARG ASP TYR LEU ARG ARG PHE THR ARG LEU GLU PHE ILE PRO LEU VAL

ILE TYR ASN ALA ALA GLN ASP HIS THR VAL VAL ARG VAL LEU ARG PRO SER PHE GLU GLN ASP HIS SER ARG LEU VAL LEU GLU ASP GLU PHE PRO THR PHE LEU TYR ASP GLN ASP ASP ASN SER ALA ASP ILE ALA ALA SER GLY ALA ALA PRO THR PRO PRO VAL

PRO PHE ASN ARG VAL PRO VAL ASN ILE GLN PHE LEU ARG GLU GLU ASN PRO PRO PRO ILE ALA ARG VAL GLN LEU PRO PRO ARG ARG HIS ARG HIS ARG ALA ALA ALA ALA ASP ASP GLY ILE LEU ASP HIS VAL GLN LEU ASP ASP ASP THR THR ARG THR ALA ASP SER GLY LEU VAL LEU SER

THR ALA PHE GLY SER VAL PHE GLN GLU ASN ARG LEU GLY GLU THR PRO LEU CYS ARG ASP GLU GLU GLU GLU GLN GLN PHE ALA SER PRO PRO ILE THR VAL LEU THR GLN ASN VAL LEU SER ALA LEU GLU ILE LEU GLU ARG LEU VAL ARG LEU ASP

• Molecule 3: Triplex capsid protein 1

Chain g:

MET ASP ALA ARG ALA VAL ALA LYS ARG PRO ARG ASP PRO ALA ASP GLU ASP ASN GLU LEU VAL THR ALA LEU LYS ALA LYS ARG GLU VAL ASN THR ILE SER VAL ARG TYR LEU TYR HIS ALA ASP HIS Q44 F51 G55 F59 E60 A61 C74 D75 S76 L80 G88

A91 S95 C100 L101 L102 E103 R112 A113 Q116 D119 L125 L140 T143 L154 TYR ASN THR LEU LYS THR GLU VAL PHE ALA L165 E176 D194 E197 T198 R199 K267 E268 L269 G284 D285 V290

• Molecule 3: Triplex capsid protein 1

Chain m: [100%]

M1 D75 I142 E177 P196 E197 V290

• Molecule 4: Capsid vertex component 1

Chain M: [16%] [79%] [21%]

M1 E12 A16 D17 Q29 E30 V31 L32 E35 D49 S50 A51 G52 R53 A58 P59 G60 G61 D62 E63 D64 S69 D70 D74 R80 A81 E102 L103 L104 Q109 E117 K118 E119 Q120 R121 G133 D138 R166 R170 E171 E172 M173 E174 A175

N176 LYS ARG ASP ARG GLN HIS GLN LEU ALA THR THR THR ASN HIS ARG ARG ARG GLY GLY LEU ARG ASN ASN LEU ASP ASN GLY SER ASP ARG ARG LEU PRO GLU ALA ALA VAL ALA SER LEU GLU THR ALA VAL SER THR PRO PHE GLU ILE PRO ASN GLY ALA GLY THR SER SER

ALA ASN GLY ASP ARG PHE SER ASN LEU GLU GLN ARG VAL ALA ARG LEU LEU ARG GLY LEU ASP GLU GLU PHE ILE TYR HIS ALA GLY LEU PRO LEU GLU PRO PRO SER LYS ILE ARG GLY HIS GLU LEU VAL GLN LEU ARG LEU ASP ASP VAL ASN PRO ASP LEU MET TYR ALA THR ASP PRO HIS

ASP R297 D298 E299 V300 A301 R315 D319 R325 E340 E347 V348 R352 D355 A356 Y357 R358 A359 R360 I361 A362 R369 A370 D373 R381 G384 A385 S399 R408 D416 R421 I424 A436 R444 R445 Q446 R447 S450 A461 E456

G460 P461 R462 N463 E464 SER GLY PRO P468 A469 R479 R498 D506 R507 R510 R513 E519 D528 R544 H548 G549 D557 N561 F562 E563 A564 E573 A574 G575 R576 Q577 E580 P590 F591 ASP ASP LEU

• Molecule 5: Capsid vertex component 2

Chain N: [10%] [90%]

MET SER LEU LEU HIS THR PHE TRP ARG LEU PRO VAL A13 C26 P27 E28 R29 V30 L31 R32 R33 L34 D37 A38 A39 V40 T41 M42 R43 G44 G45 R46 R55 K58 L61 R62 Q63 R66 D67 L68 G69 H70 R71 V72 Q73 T74 Y75 C76 E77 ASP LEU GLY ARG

VAL SER GLU GLU ALA GLU ALA LEU LEU ASN GLN GLN CYS GLU LEU ASP GLU GLY PRO SER PRO ARG THR LEU LEU GLN PRO PRO CYS ARG PRO ARG SER SER SER PRO GLY THR GLY VAL VAL ALA GLY ALA SER ALA VAL PRO HIS GLY LEU TYR SER ARG HIS ASP ALA ILE THR GLY PRO ALA

ALA ALA PRO SER ASP VAL VAL ALA PRO SER ASP ALA VAL ALA ALA SER ALA ALA ALA GLY ALA SER SER THR TRP LEU ALA GLN CYS ALA GLU ARG PRO LEU PRO GLY ASN VAL PRO SER TYR PHE GLY ILE THR GLN ASN ASP PRO PHE ILE ARG PHE HIS THR ASP PHE ARG GLY GLU

VAL VAL ASN THR MET PHE GLU ASN ALA SER THR TRP THR PHE SER GLY ILE TRP TYR ARG LEU LYS ARG GLY LEU TYR LEU ALA GLN ASP ASN PHE SER ILE SER GLN GLU LEU LEU GLY VAL VAL ASN ALA LEU GLU

WORLDWIDE
wwPDB
PROTEIN DATA BANK

• Molecule 5: Capsid vertex component 2

Chain O:

5%

11%

89%

• Molecule 6: ORFL92C_UL32

Chain 1:

• Molecule 7: Small capsomere-interacting protein

Chain R:

• Molecule 7: Small capsomere-interacting protein

Chain S:

17%

83%   16%

• Molecule 7: Small capsomere-interacting protein

Chain T:

57%

83%   16%

• Molecule 7: Small capsomere-interacting protein

Chain i:

40%

84%   16%

• Molecule 7: Small capsomere-interacting protein

Chain j:

25%

83%   16%

• Molecule 8: Major capsid protein

Chain a:

94%   6%

N1184 S1197 T1307 E1308 G1342 F1368 N1369 S1370

• Molecule 8: Major capsid protein

Chain B: 97%

M1 A104 R204 A225 D237 F305 VAL LEU SER PRO GLU ASN ALA VAL THR ALA ILE SER HIS SER ILE LEU A323 S345 GLN ALA GLY ALA H350 D418 D444 A445 L446 E456 E480 G489 R493 R503 D563 E592 D614 G619

H640 D663 G664 A665 G692 E700 R736 L739 N740 P741 A742 E745 R756 A759 M760 D761 A762 D763 D769 N803 L804 D810 L811 A822 A823 T824 ALA VAL SER THR SER GLY THR THR SER LYS GLU SER THR SER GLY VAL THR P842 E843 D844

G854 E859 E862 D863 A868 H869 Q874 E878 E888 L917 K928 D954 D955 R1139 R1159 L1176 N1184 D1296 C1303 G1340 F1368 N1369 S1370

• Molecule 8: Major capsid protein

Chain C: 97%

M1 G14 ILE PRO THR ASP PHE LEU THR HIS VAL LYS THR SER ALA GLY GLU GLU M31 Y38 TYR GLY ASP D42 R204 F219 S265 L362 D441 M488 G489 G490 A491 E572 D589 Y590 E591 D614 A623 E659 D663 G664 A665 R682

E728 N740 P741 A742 N743 S752 A759 D763 D769 R772 D776 L800 L811 A822 A823 THR ALA VAL SER THR SER GLY THR THR SER LYS GLU SER THR SER GLY VAL THR PRO GLU ASP S845 A848 Q851 E855 E859 E862 D863 A868

H869 E878 D909 E932 V937 R958 A980 D1040 R1139 M1181 N1184 A1289 T1307 F1368 N1369 S1370

• Molecule 8: Major capsid protein

Chain D: 6%   94%   5%

MET GLU ASN TRP SER ALA LEU GLU LEU LEU LEU PRO LYS VAL GLY ILE ILE PRO THR ASP PHE LEU THR HIS VAL LYS THR SER ALA GLY GLU GLU MET PHE GLU ALA LEU ARG ILE TYR TYR GLY ASP ASP PRO GLU ARG TYR ASN ILE HIS F50 A104 A134 T137 Y138 E141 T142

F143 E144 G145 T146 I147 L148 D149 K150 A203 D418 D444 A445 L446 E456 P487 R493 R503 D515 E544 D563 D589 R595 L609 D614 L625 R628 L644 E659 D663 E728 L739 N740 N743 I744 H748 S752

L757 G758 D761 A762 D763 E764 R772 K805 L808 P821 ALA ALA THR ALA VAL SER THR SER GLY THR THR SER LYS GLU SER THR SER GLY VAL THR PRO GLU ASP SER I846 E855 E862 D863 V864 A865 T866 D867 A868 H869 Q874 A875 E878 L881

G887 K928 E932 A951 D954 E962 N1000 D1070 I1071 D1112 L1142 L1143 D1144 T1147 M1156 L1174 N1184 D1216 E1250 S1256 A1331 F1368 N1369 S1370

• Molecule 8: Major capsid protein

Chain Y:

9%

98%

M1 D82 P309 E310 N311 A312 V313 T314 A315 I316 S317 Y318 D390 D418 D444 Q485 E486 P487 M488 G489 G490 R493 R494 H497 R500 V501 D520 E544 N545 S546 E547 R585 D589 Y590 E591 D614 D622 L625 L644 L645 A679

G692 A699 E728 A734 D735 R736 Q737 P738 L739 N740 P741 A742 N743 I744 E745 A746 R747 H748 H749 G750 V751 S752 D753 V754 P755 R756 L757 G758 A759 M760 D761 A762 D763 E764 P765 L766 F767 V768 D769 D770 D776 L802 K805 T806 L807 L808 V809 D810 L811 F812 Y813 R814 P815 A816

F817 L818 L819 M820 P821 ALA ALA THR ALA VAL SER THR SER GLY THR THR SER LYS GLU SER THR SER GLY VAL THR PRO GLU ASP S845 I846 A852 E855 E859 L860 D863 D867 A868 H869 T870 Q874 E878 L879 F880 L881 Q884 G887 E888 K891 H915

I931 E932 A950 D970 L1002 D1112 E1138 A1163 N1184 L1239 D1296 E1320 A1341 E1358 F1368 N1369 S1370

• Molecule 8: Major capsid protein

Chain Z:

6%

97%

M1 E403 D418 E466 S471 E472 PRO ALA MET GLN ARG LEU LEU GLU CYS ARG PHE GLN GLN E486 G490 A491 R500 R503 D515 D589 G619 D622 A632 A652 D663 G664 A665 E700 M727 R736 N740 P741 A742 N743 R747

H748 S752 D753 A759 D763 E764 D769 L800 K805 D810 M820 P821 A822 A823 T824 ALA VAL SER THR SER GLY THR THR SER LYS GLU SER THR SER GLY VAL THR PRO GLU ASP S845 R850 E859 L860 D867 A868 H869 L873 Q874 A875 E878 L879

F880 L881 E888 L935 P936 V937 D954 D955 G1107 Q1141 L1142 L1143 D1144 T1145 E1146 T1147 I1148 S1149 M1150 L1151 T1152 F1153 K1169 M1181 N1184 H1217 R1247 E1250 E1269 D1283 D1298 V1304 F1368 N1369 S1370

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23136	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 $(e^-/\text{Å}^2)$	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	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	I	0.29	0/2304	0.58	1/3125 (0.0%)
1	h	0.29	0/2302	0.60	1/3128 (0.0%)
1	n	0.29	0/2366	0.58	0/3212
1	o	0.30	0/2279	0.57	0/3092
2	H	0.29	0/174	0.56	0/233
2	P	0.28	0/174	0.50	0/233
3	g	0.29	0/1936	0.55	0/2625
3	m	0.30	0/2374	0.56	0/3221
4	M	0.30	0/3935	0.57	0/5331
5	N	0.31	0/560	0.60	0/751
5	O	0.29	0/600	0.62	1/808 (0.1%)
6	1	0.30	0/2366	0.59	1/3192 (0.0%)
7	R	0.26	0/520	0.58	0/697
7	S	0.28	0/520	0.56	0/697
7	T	0.28	0/520	0.61	1/697 (0.1%)
7	i	0.30	0/520	0.65	0/697
7	j	0.30	0/520	0.55	0/697
8	B	0.30	0/10819	0.55	3/14733 (0.0%)
8	C	0.30	0/10790	0.54	2/14695 (0.0%)
8	D	0.30	0/10513	0.56	3/14322 (0.0%)
8	Y	0.30	0/10932	0.55	2/14892 (0.0%)
8	Z	0.30	0/10835	0.55	1/14762 (0.0%)
8	a	0.31	0/10410	0.56	0/14183
All	All	0.30	0/88269	0.56	16/120023 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	1	0	1
8	Y	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	a	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	h	119	LEU	CA-CB-CG	7.92	133.51	115.30
7	T	53	LEU	CA-CB-CG	6.74	130.80	115.30
8	D	1156	MET	CA-CB-CG	5.61	122.84	113.30
8	C	362	LEU	CA-CB-CG	5.48	127.91	115.30
8	Y	1002	LEU	CA-CB-CG	5.47	127.89	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1	69	HIS	Peptide
8	Y	585	ARG	Peptide
8	a	585	ARG	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	I	279/306 (91%)	264 (95%)	15 (5%)	0	100	100
1	h	281/306 (92%)	262 (93%)	19 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	289/306 (94%)	267 (92%)	22 (8%)	0	100	100
1	o	276/306 (90%)	263 (95%)	13 (5%)	0	100	100
2	H	18/2241 (1%)	17 (94%)	1 (6%)	0	100	100
2	P	18/2241 (1%)	17 (94%)	1 (6%)	0	100	100
3	g	233/290 (80%)	214 (92%)	19 (8%)	0	100	100
3	m	288/290 (99%)	273 (95%)	15 (5%)	0	100	100
4	M	462/594 (78%)	432 (94%)	30 (6%)	0	100	100
5	N	63/642 (10%)	61 (97%)	2 (3%)	0	100	100
5	O	65/642 (10%)	64 (98%)	1 (2%)	0	100	100
6	1	283/1048 (27%)	270 (95%)	13 (5%)	0	100	100
7	R	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
7	S	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	T	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	i	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	j	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
8	B	1324/1370 (97%)	1245 (94%)	79 (6%)	0	100	100
8	C	1322/1370 (96%)	1244 (94%)	78 (6%)	0	100	100
8	D	1293/1370 (94%)	1228 (95%)	65 (5%)	0	100	100
8	Y	1343/1370 (98%)	1254 (93%)	89 (7%)	0	100	100
8	Z	1331/1370 (97%)	1252 (94%)	79 (6%)	0	100	100
8	a	1280/1370 (93%)	1192 (93%)	88 (7%)	0	100	100
All	All	10753/17807 (60%)	10113 (94%)	640 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2　Protein sidechains ⓘ

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	I	257/273 (94%)	257 (100%)	0	100	100
1	h	256/273 (94%)	255 (100%)	1 (0%)	89	91
1	n	262/273 (96%)	262 (100%)	0	100	100
1	o	254/273 (93%)	253 (100%)	1 (0%)	89	91
2	H	19/1941 (1%)	19 (100%)	0	100	100
2	P	19/1941 (1%)	19 (100%)	0	100	100
3	g	207/252 (82%)	207 (100%)	0	100	100
3	m	252/252 (100%)	252 (100%)	0	100	100
4	M	395/500 (79%)	394 (100%)	1 (0%)	91	92
5	N	58/526 (11%)	58 (100%)	0	100	100
5	O	64/526 (12%)	64 (100%)	0	100	100
6	1	256/883 (29%)	256 (100%)	0	100	100
7	R	59/68 (87%)	58 (98%)	1 (2%)	56	72
7	S	59/68 (87%)	58 (98%)	1 (2%)	56	72
7	T	59/68 (87%)	59 (100%)	0	100	100
7	i	59/68 (87%)	59 (100%)	0	100	100
7	j	59/68 (87%)	58 (98%)	1 (2%)	56	72
8	B	1162/1192 (98%)	1160 (100%)	2 (0%)	92	94
8	C	1158/1192 (97%)	1153 (100%)	5 (0%)	89	91
8	D	1130/1192 (95%)	1128 (100%)	2 (0%)	92	94
8	Y	1174/1192 (98%)	1168 (100%)	6 (0%)	86	90
8	Z	1163/1192 (98%)	1160 (100%)	3 (0%)	91	92
8	a	1120/1192 (94%)	1118 (100%)	2 (0%)	92	94
All	All	9501/15405 (62%)	9475 (100%)	26 (0%)	90	92

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	C	958	ARG
8	Y	82	ASP
8	Z	1169	LYS
8	D	1368	PHE
8	Y	418	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129

such sidechains are listed below:

Mol	Chain	Res	Type
8	Z	214	ASN
8	Z	534	HIS
8	B	749	HIS
8	B	618	HIS
8	Z	849	GLN

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-31297. 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
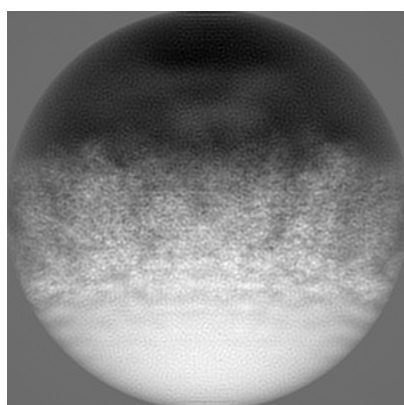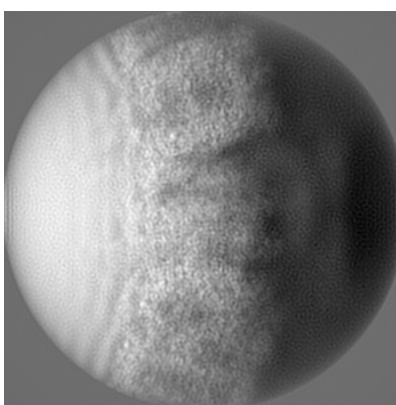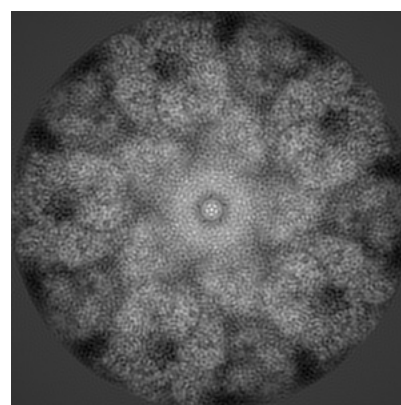
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
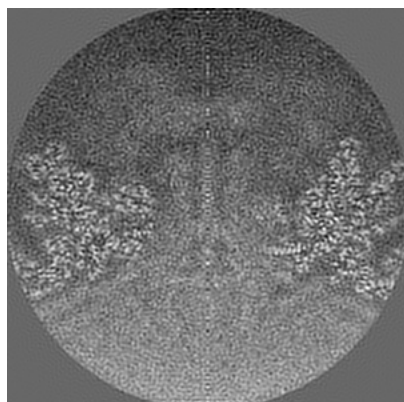
6.2.1 Primary map
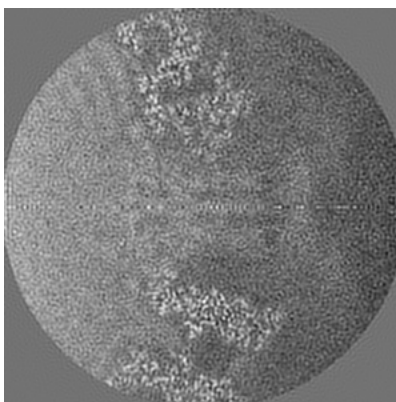
X Index: 128   Y Index: 128   Z Index: 128
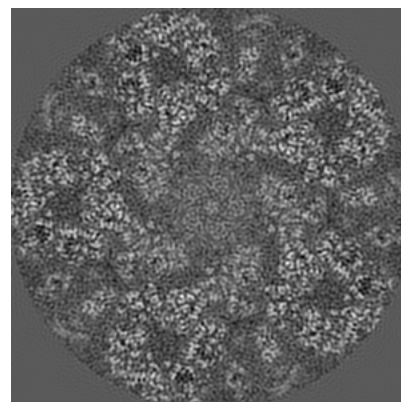
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
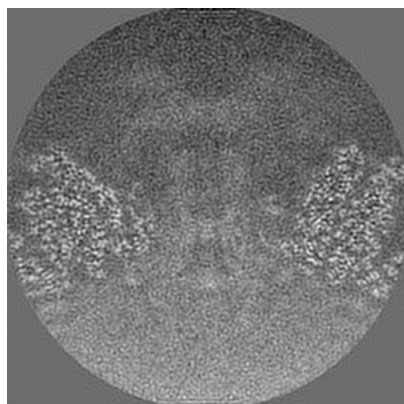
6.3.1 Primary map
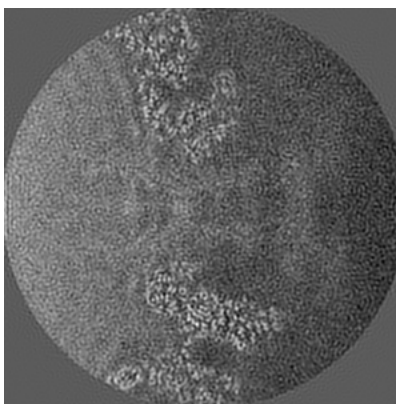
| X Index: 123 | Y Index: 123 | Z Index: 101 |
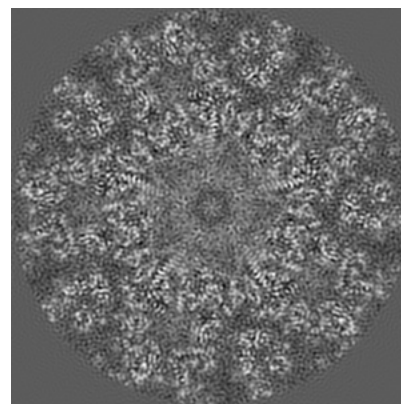
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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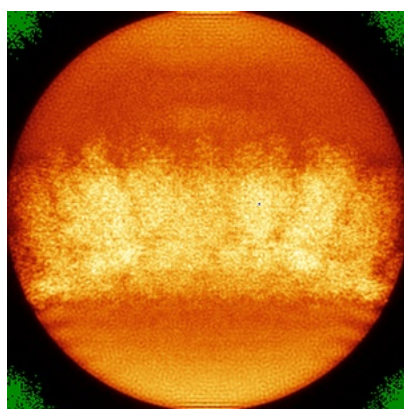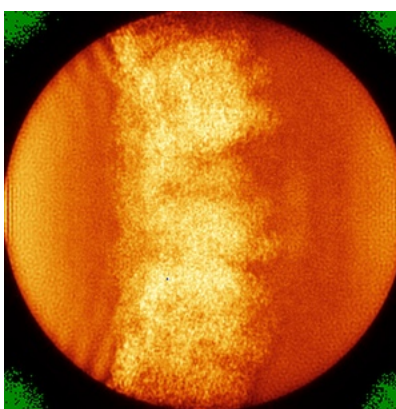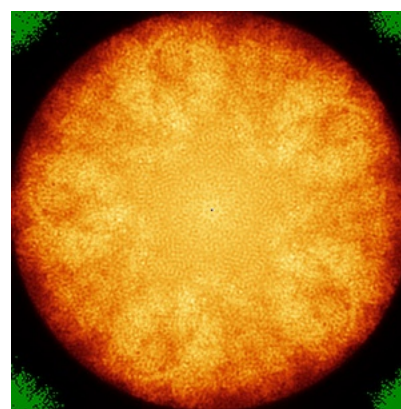
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
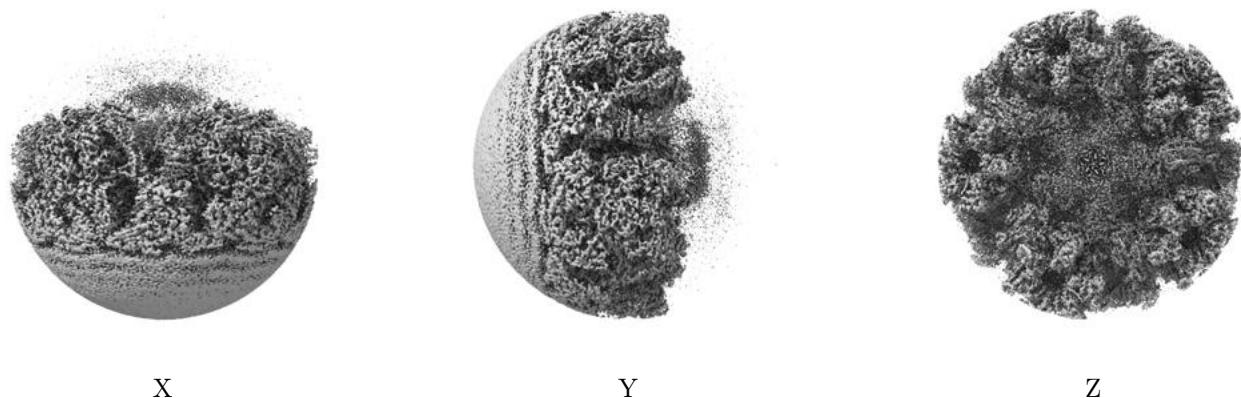
The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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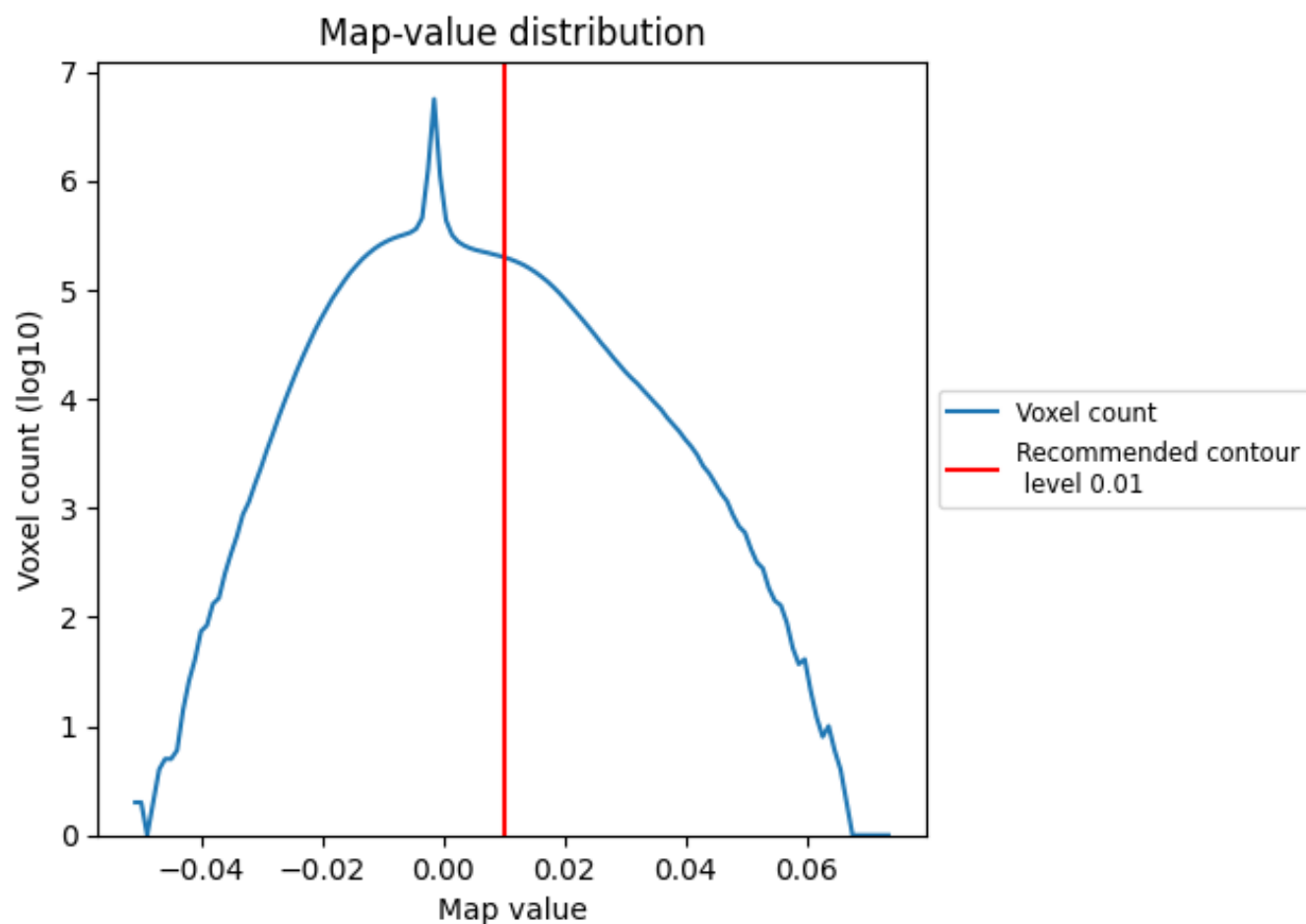
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
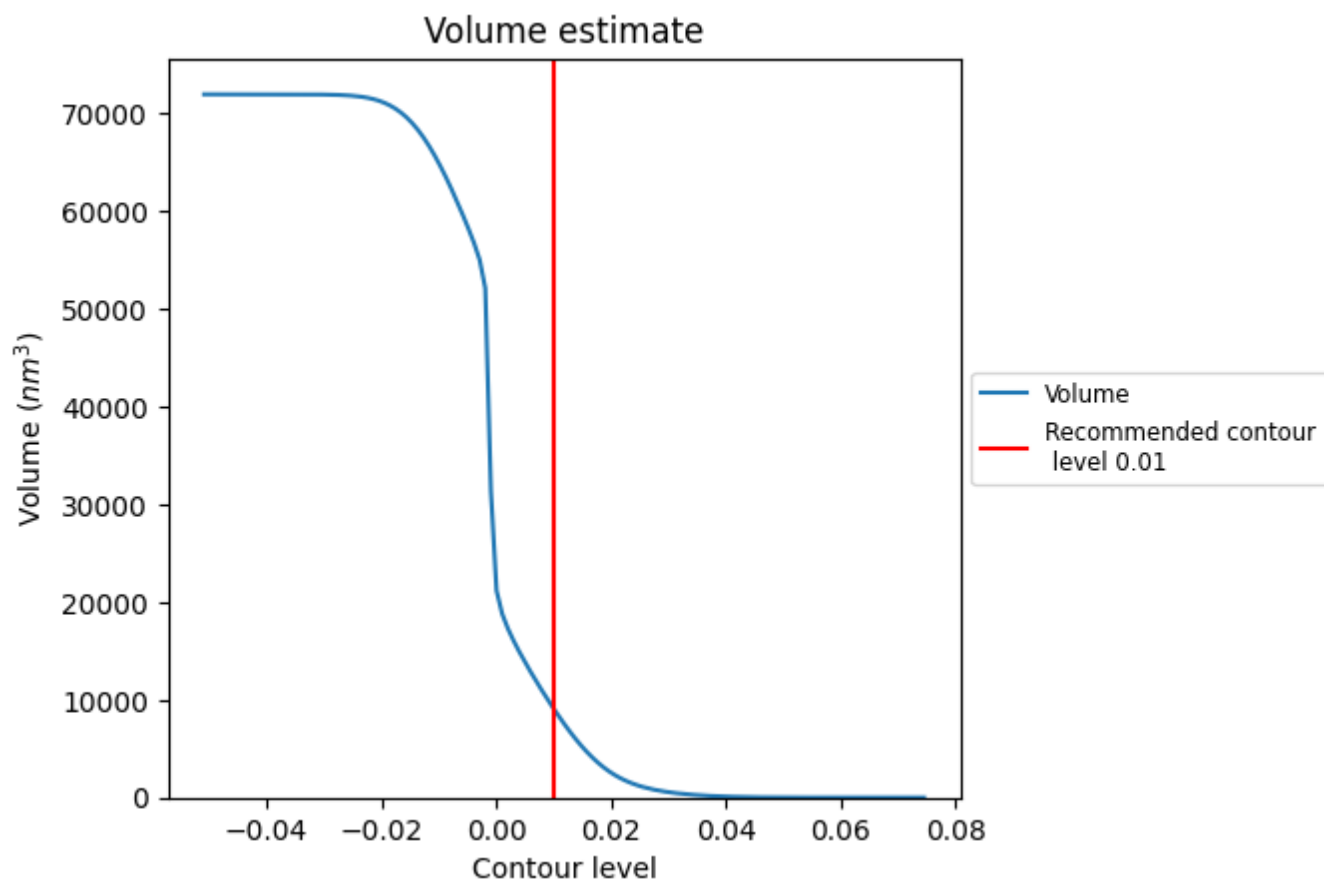
Volume estimate

The volume at the recommended contour level is 9110 nm^3; this corresponds to an approximate mass of 8230 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 ⓘ
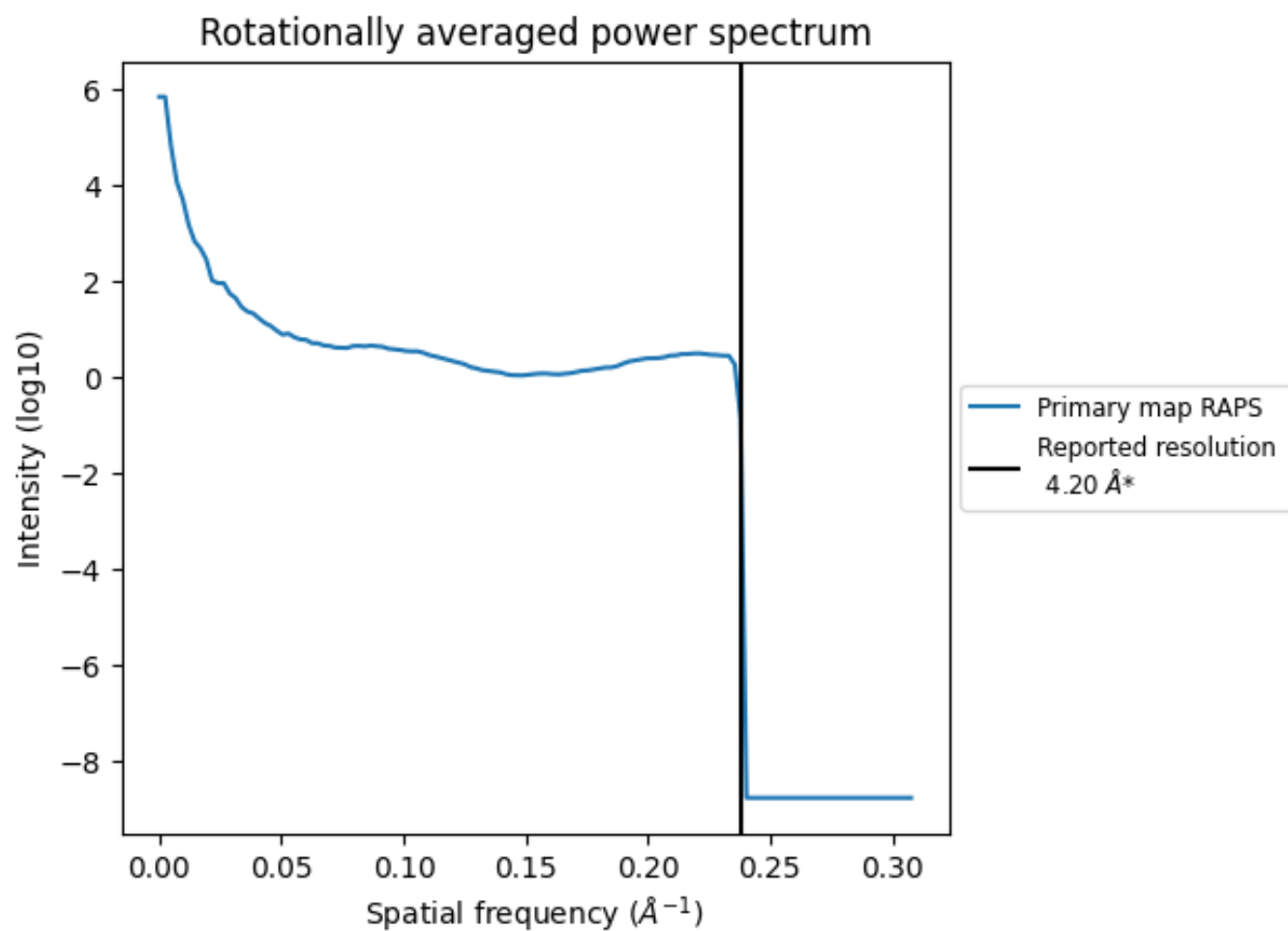
*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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-31297 and PDB model 7ET3. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ

| X | Y | Z |
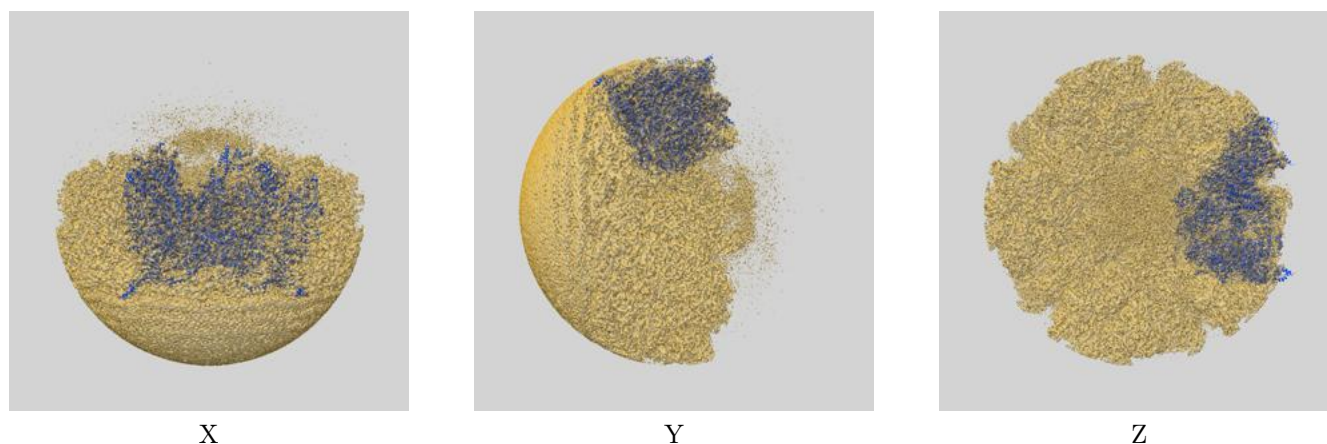
9.1.2 Map-model assembly overlay ⓘ

| X | Y | Z |
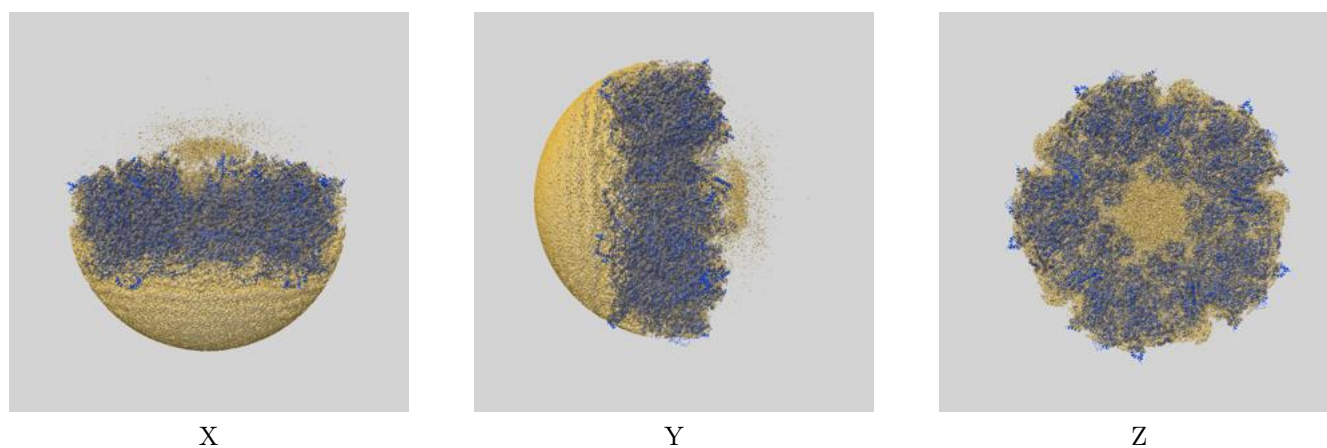
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X   Y   Z
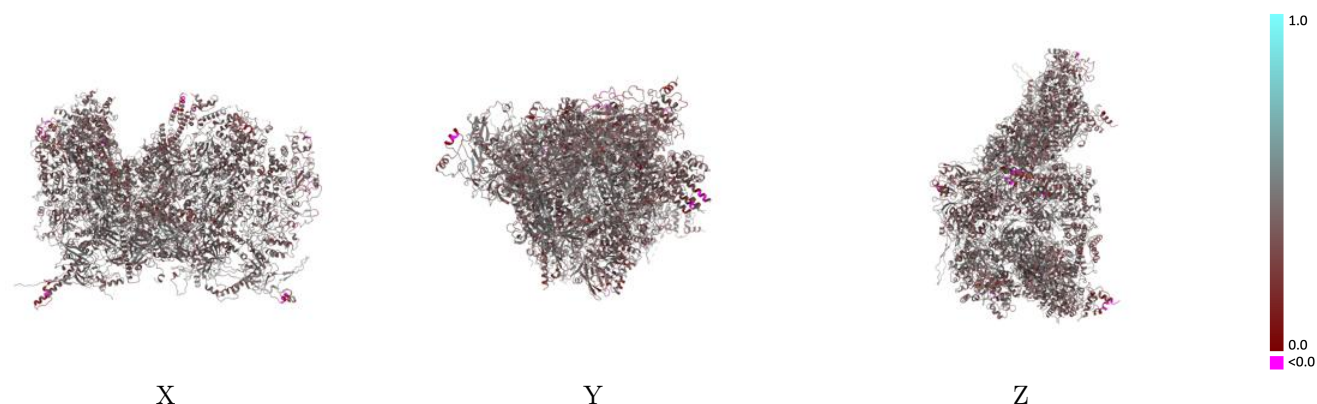
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
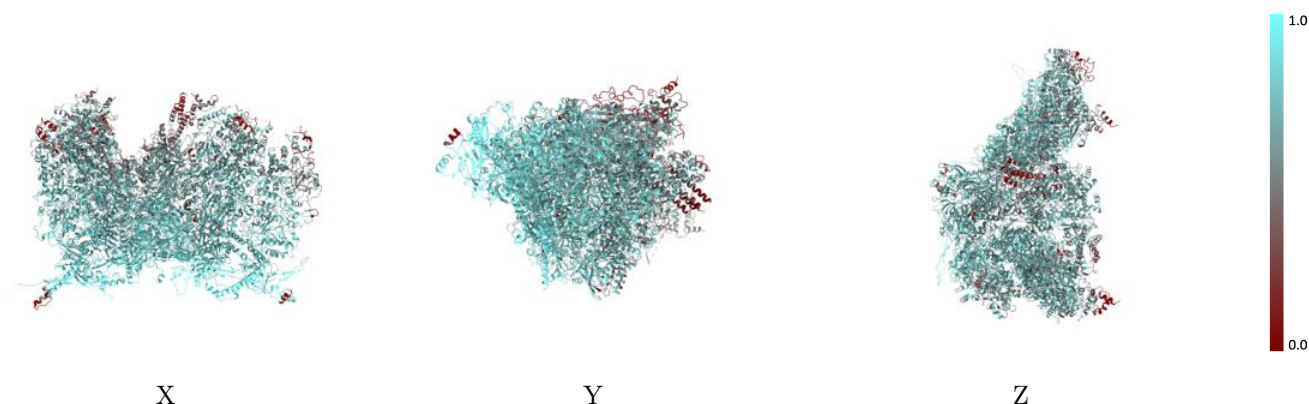
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4　Atom inclusion　ⓘ
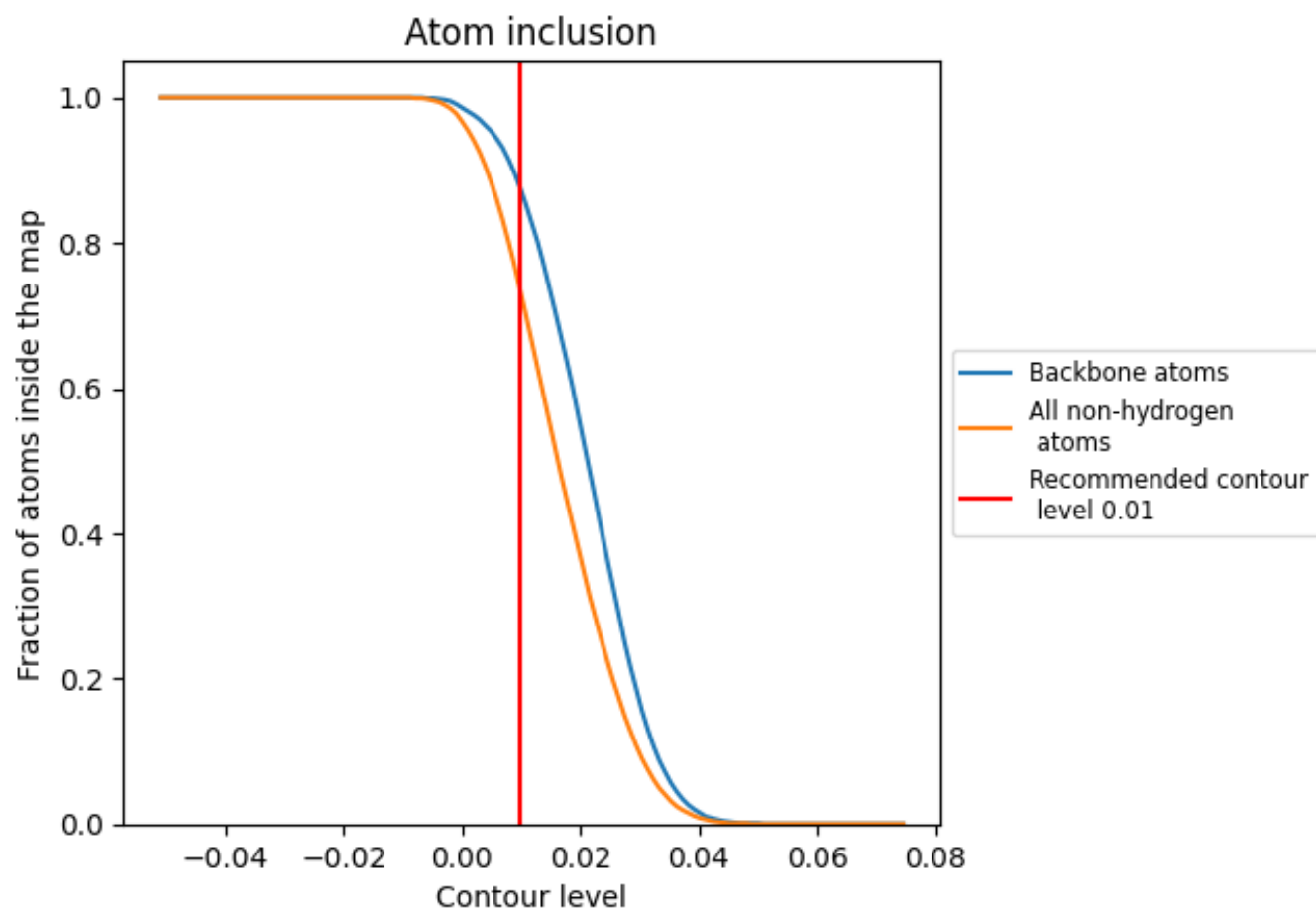
At the recommended contour level, 87% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.3980
1	0.5500	0.3720
B	0.7680	0.4060
C	0.7790	0.4130
D	0.7550	0.4000
H	0.2870	0.3060
I	0.7260	0.3830
M	0.6010	0.3910
N	0.4520	0.3440
O	0.3990	0.3210
P	0.2640	0.2900
R	0.4780	0.3630
S	0.5200	0.3800
T	0.2790	0.2660
Y	0.7390	0.3930
Z	0.7650	0.4070
a	0.7750	0.4090
g	0.6770	0.3630
h	0.7020	0.3750
i	0.3590	0.3420
j	0.4900	0.3610
m	0.8030	0.4100
n	0.7570	0.4000
o	0.7730	0.4000

1.0

0.0
<0.0