



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2025 – 03:30 am BST

PDB ID : 9GB7 / pdb_00009gb7
EMDB ID : EMD-51200
Title : Extended phiCD508 neck
Authors : Wilson, J.S.; Fagan, R.P.; Bullough, P.A.
Deposited on : 2024-07-29
Resolution : 3.40 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

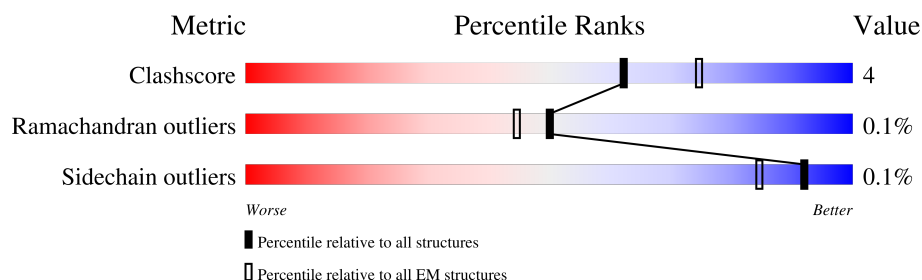
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	210492	15764
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 $\leq 5\%$. 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	137	 88% 7% 5%
1	B	137	 88% 7% 5%
1	C	137	 88% 7% 5%
1	D	137	 85% 9% 5%
1	E	137	 85% 10% 5%
1	F	137	 87% 8% 5%
2	G	125	 92% 7% .
2	K	125	 90% 9% .

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Mol	Chain	Length	Quality of chain
2	M	125	 90% 10% .
2	O	125	 88% 11% .
2	Q	125	 89% 10% .
2	X	125	 89% 10% .
3	H	273	 87% 13%
3	L	273	 88% 11%
3	N	273	 89% 11%
3	P	273	 88% 12%
3	R	273	 87% 13%
3	d	273	 100%
4	I	112	 84% 8% 5% 8%
4	J	112	 87% 5% 7% 8%
4	S	112	 83% 9% 8%
4	T	112	 81% 11% 6% 8%
4	U	112	 83% 9% 5% 8%
4	V	112	 87% 5% 8%
4	W	112	 86% 6% 8%
4	Y	112	 88% . 8%
4	Z	112	 88% . 8%
4	a	112	 92% 8% 7%
4	b	112	 92% 8% 7%
4	c	112	 92% 8% 7%
5	e	473	 89% 11% 49%
5	f	473	 89% 11% 48%
5	g	473	 89% 11% 48%

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Mol	Chain	Length	Quality of chain		
5	h	473	48%	88%	11%
5	i	473	49%	89%	11%
5	j	473	48%	89%	11%
6	k	500	9%	89%	11%
6	l	500	10%	89%	11%
6	m	500	10%	89%	11%
6	n	500	9%	89%	11%
6	o	500	10%	89%	11%
6	p	500	10%	89%	11%
6	q	500	9%	89%	11%
6	r	500	10%	89%	11%
6	s	500	10%	89%	11%
6	t	500	10%	89%	11%
6	u	500	10%	89%	11%
6	v	500	10%	89%	11%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 193656 atoms, of which 96468 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 gp56 - Tail tube protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	130	Total	C	H	N	O	S	0	0
			2060	652	1031	167	207	3		
1	B	130	Total	C	H	N	O	S	0	0
			2060	652	1031	167	207	3		
1	C	130	Total	C	H	N	O	S	0	0
			2060	652	1031	167	207	3		
1	D	130	Total	C	H	N	O	S	0	0
			2060	652	1031	167	207	3		
1	E	130	Total	C	H	N	O	S	0	0
			2060	652	1031	167	207	3		
1	F	130	Total	C	H	N	O	S	0	0
			2060	652	1031	167	207	3		

- Molecule 2 is a protein called gp51 - Neck valve protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	124	Total	C	H	N	O	S	0	0
			2019	623	1021	172	197	6		
2	K	124	Total	C	H	N	O	S	0	0
			2019	623	1021	172	197	6		
2	M	124	Total	C	H	N	O	S	0	0
			2019	623	1021	172	197	6		
2	O	124	Total	C	H	N	O	S	0	0
			2019	623	1021	172	197	6		
2	Q	124	Total	C	H	N	O	S	0	0
			2019	623	1021	172	197	6		
2	X	124	Total	C	H	N	O	S	0	0
			2019	623	1021	172	197	6		

- Molecule 3 is a protein called gp53 - Tail adaptor protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	272	Total	C	H	N	O	S	0	0
			4462	1397	2247	380	426	12		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	272	Total	C	H	N	O	S	0	0
			4462	1397	2247	380	426	12		
3	N	272	Total	C	H	N	O	S	0	0
			4462	1397	2247	380	426	12		
3	P	272	Total	C	H	N	O	S	0	0
			4462	1397	2247	380	426	12		
3	R	272	Total	C	H	N	O	S	0	0
			4462	1397	2247	380	426	12		
3	d	272	Total	C	H	N	O	S	0	0
			4462	1397	2247	380	426	12		

- Molecule 4 is a protein called gp50 - Portal adaptor protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	I	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	J	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	S	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	T	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	U	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	V	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	W	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	Y	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	Z	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	a	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	b	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		
4	c	103	Total	C	H	N	O	S	0	0
			1649	528	816	129	170	6		

- Molecule 5 is a protein called gp55 - Tail sheath protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	e	420	Total	C	H	N	O	S	0	0
			6585	2089	3289	529	668	10		
5	f	420	Total	C	H	N	O	S	0	0
			6585	2089	3289	529	668	10		
5	g	420	Total	C	H	N	O	S	0	0
			6585	2089	3289	529	668	10		
5	h	420	Total	C	H	N	O	S	0	0
			6585	2089	3289	529	668	10		
5	i	420	Total	C	H	N	O	S	0	0
			6585	2089	3289	529	668	10		
5	j	420	Total	C	H	N	O	S	0	0
			6585	2089	3289	529	668	10		

- Molecule 6 is a protein called gp45 - Portal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	l	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	m	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	n	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	o	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	p	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	q	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	r	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	s	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	t	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	u	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		
6	v	445	Total	C	H	N	O	S	0	0
			6926	2235	3429	579	668	15		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	51	ASN	LYS	conflict	UNP A0A069A478
k	419	CYS	SER	conflict	UNP A0A069A478
k	456	ARG	ILE	conflict	UNP A0A069A478
k	457	GLU	VAL	conflict	UNP A0A069A478
l	51	ASN	LYS	conflict	UNP A0A069A478
l	419	CYS	SER	conflict	UNP A0A069A478
l	456	ARG	ILE	conflict	UNP A0A069A478
l	457	GLU	VAL	conflict	UNP A0A069A478
m	51	ASN	LYS	conflict	UNP A0A069A478
m	419	CYS	SER	conflict	UNP A0A069A478
m	456	ARG	ILE	conflict	UNP A0A069A478
m	457	GLU	VAL	conflict	UNP A0A069A478
n	51	ASN	LYS	conflict	UNP A0A069A478
n	419	CYS	SER	conflict	UNP A0A069A478
n	456	ARG	ILE	conflict	UNP A0A069A478
n	457	GLU	VAL	conflict	UNP A0A069A478
o	51	ASN	LYS	conflict	UNP A0A069A478
o	419	CYS	SER	conflict	UNP A0A069A478
o	456	ARG	ILE	conflict	UNP A0A069A478
o	457	GLU	VAL	conflict	UNP A0A069A478
p	51	ASN	LYS	conflict	UNP A0A069A478
p	419	CYS	SER	conflict	UNP A0A069A478
p	456	ARG	ILE	conflict	UNP A0A069A478
p	457	GLU	VAL	conflict	UNP A0A069A478
q	51	ASN	LYS	conflict	UNP A0A069A478
q	419	CYS	SER	conflict	UNP A0A069A478
q	456	ARG	ILE	conflict	UNP A0A069A478
q	457	GLU	VAL	conflict	UNP A0A069A478
r	51	ASN	LYS	conflict	UNP A0A069A478
r	419	CYS	SER	conflict	UNP A0A069A478
r	456	ARG	ILE	conflict	UNP A0A069A478
r	457	GLU	VAL	conflict	UNP A0A069A478
s	51	ASN	LYS	conflict	UNP A0A069A478
s	419	CYS	SER	conflict	UNP A0A069A478
s	456	ARG	ILE	conflict	UNP A0A069A478
s	457	GLU	VAL	conflict	UNP A0A069A478
t	51	ASN	LYS	conflict	UNP A0A069A478
t	419	CYS	SER	conflict	UNP A0A069A478
t	456	ARG	ILE	conflict	UNP A0A069A478
t	457	GLU	VAL	conflict	UNP A0A069A478
u	51	ASN	LYS	conflict	UNP A0A069A478
u	419	CYS	SER	conflict	UNP A0A069A478
u	456	ARG	ILE	conflict	UNP A0A069A478

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Chain	Residue	Modelled	Actual	Comment	Reference
u	457	GLU	VAL	conflict	UNP A0A069A478
v	51	ASN	LYS	conflict	UNP A0A069A478
v	419	CYS	SER	conflict	UNP A0A069A478
v	456	ARG	ILE	conflict	UNP A0A069A478
v	457	GLU	VAL	conflict	UNP A0A069A478

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: gp56 - Tail tube protein

Chain A: 




- Molecule 1: gp56 - Tail tube protein

Chain B: 




- Molecule 1: gp56 - Tail tube protein

Chain C: 




- Molecule 1: gp56 - Tail tube protein

Chain D: 




- Molecule 1: gp56 - Tail tube protein

Chain E: 



- Molecule 1: gp56 - Tail tube protein

Chain F:  87% 8% 5%



- Molecule 2: gp51 - Neck valve protein

Chain G:  92% 7%




- Molecule 2: gp51 - Neck valve protein

Chain K:  90% 9%




- Molecule 2: gp51 - Neck valve protein

Chain M:  90% 10%




- Molecule 2: gp51 - Neck valve protein

Chain O:  88% 11%




- Molecule 2: gp51 - Neck valve protein

Chain Q:  89% 10%




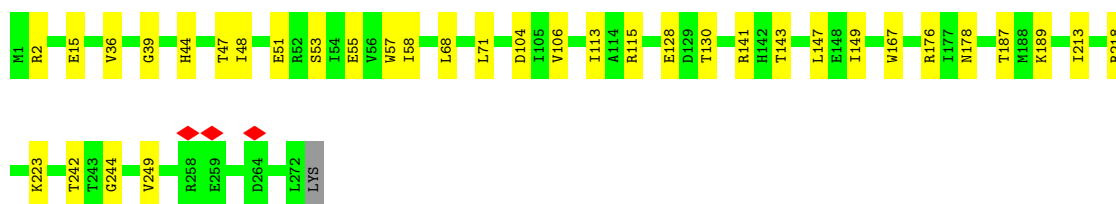
- Molecule 2: gp51 - Neck valve protein

Chain X:  89% 10%




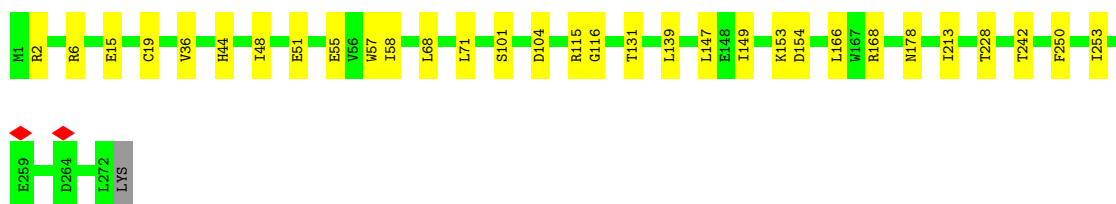
- Molecule 3: gp53 - Tail adaptor protein

Chain H:  87% 13%




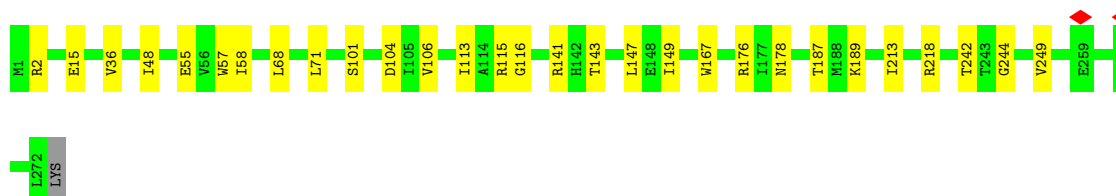
- Molecule 3: gp53 - Tail adaptor protein

Chain L:  88% 11%




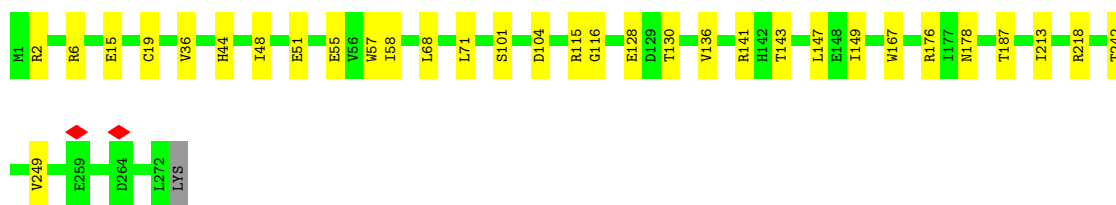
- Molecule 3: gp53 - Tail adaptor protein

Chain N:  89% 11%




- Molecule 3: gp53 - Tail adaptor protein

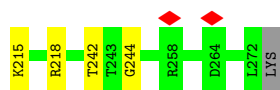
Chain P:  88% 12%



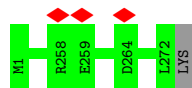
- Molecule 3: gp53 - Tail adaptor protein

Chain R:  87% 13%

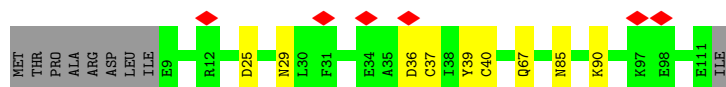
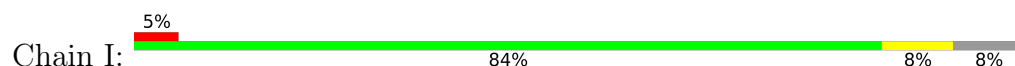




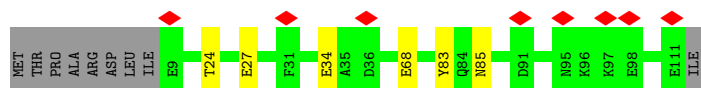
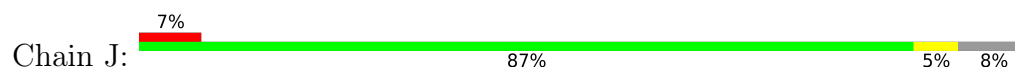
- Molecule 3: gp53 - Tail adaptor protein



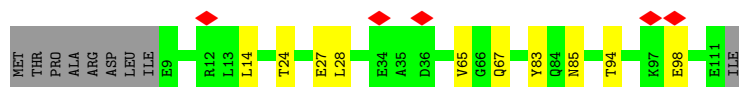
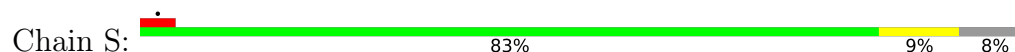
- Molecule 4: gp50 - Portal adaptor protein



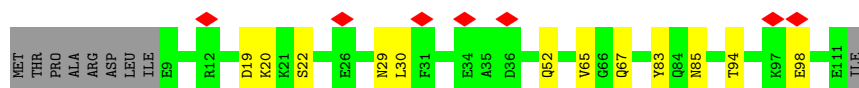
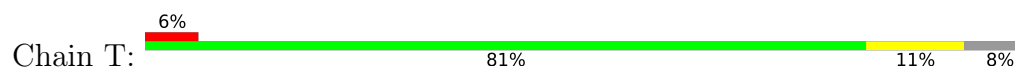
- Molecule 4: gp50 - Portal adaptor protein



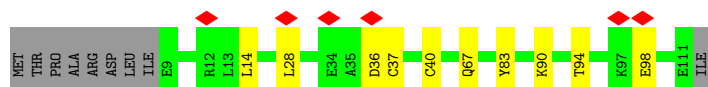
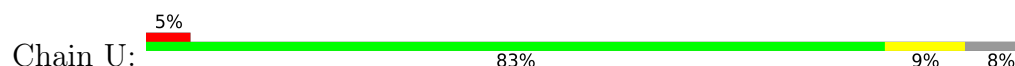
- Molecule 4: gp50 - Portal adaptor protein



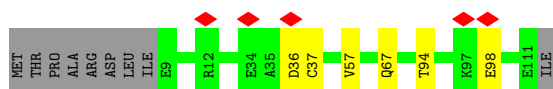
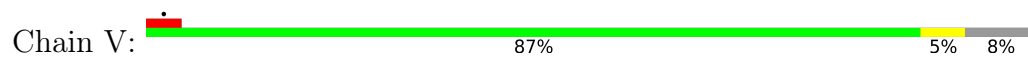
- Molecule 4: gp50 - Portal adaptor protein



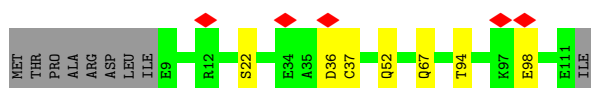
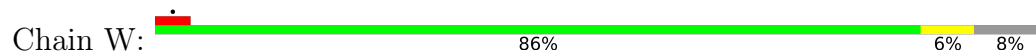
- Molecule 4: gp50 - Portal adaptor protein



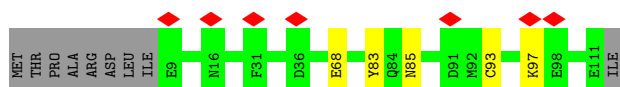
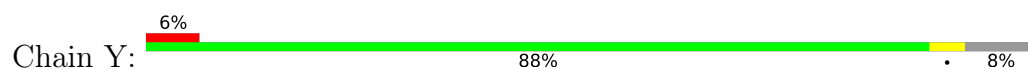
- Molecule 4: gp50 - Portal adaptor protein



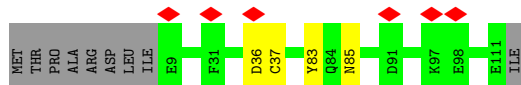
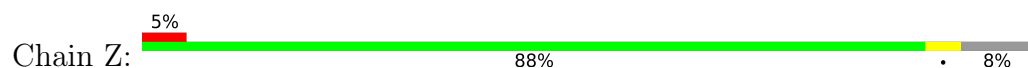
- Molecule 4: gp50 - Portal adaptor protein



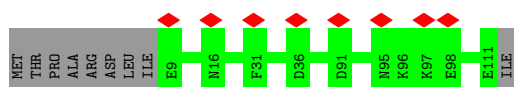
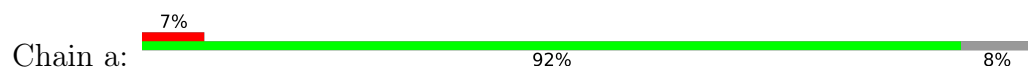
- Molecule 4: gp50 - Portal adaptor protein



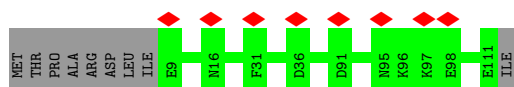
- Molecule 4: gp50 - Portal adaptor protein



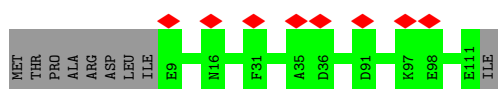
- Molecule 4: gp50 - Portal adaptor protein



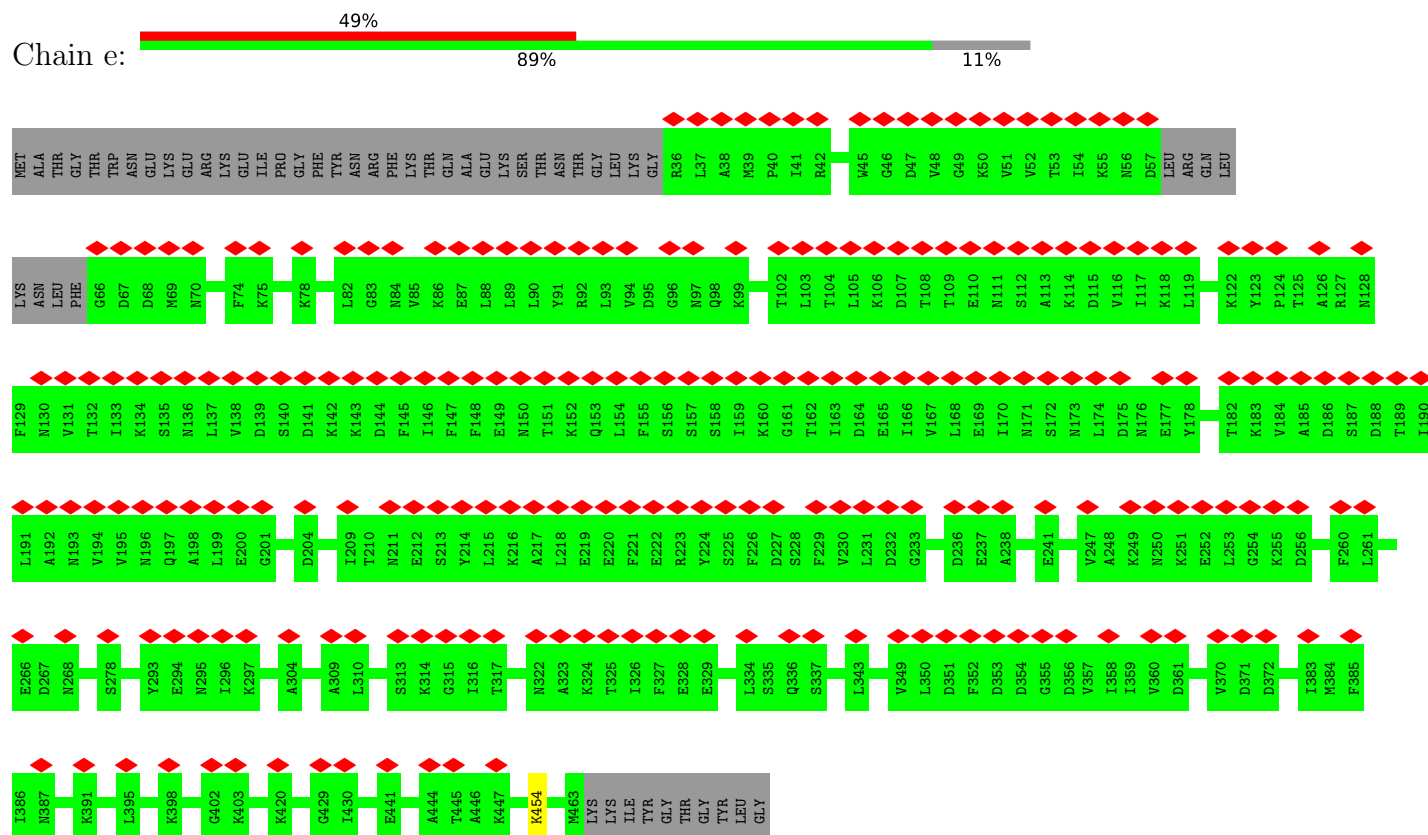
- Molecule 4: gp50 - Portal adaptor protein



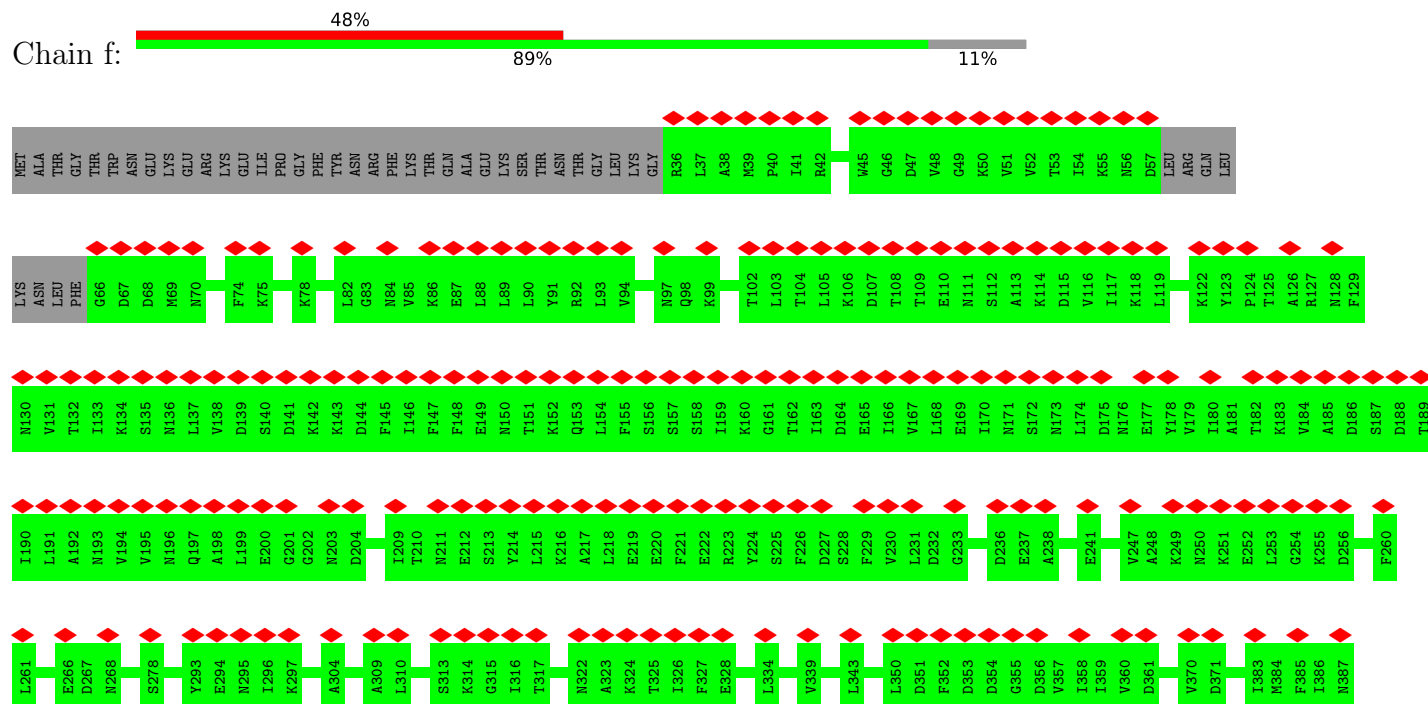
- Molecule 4: gp50 - Portal adaptor protein

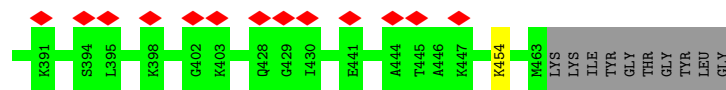


Chain e:

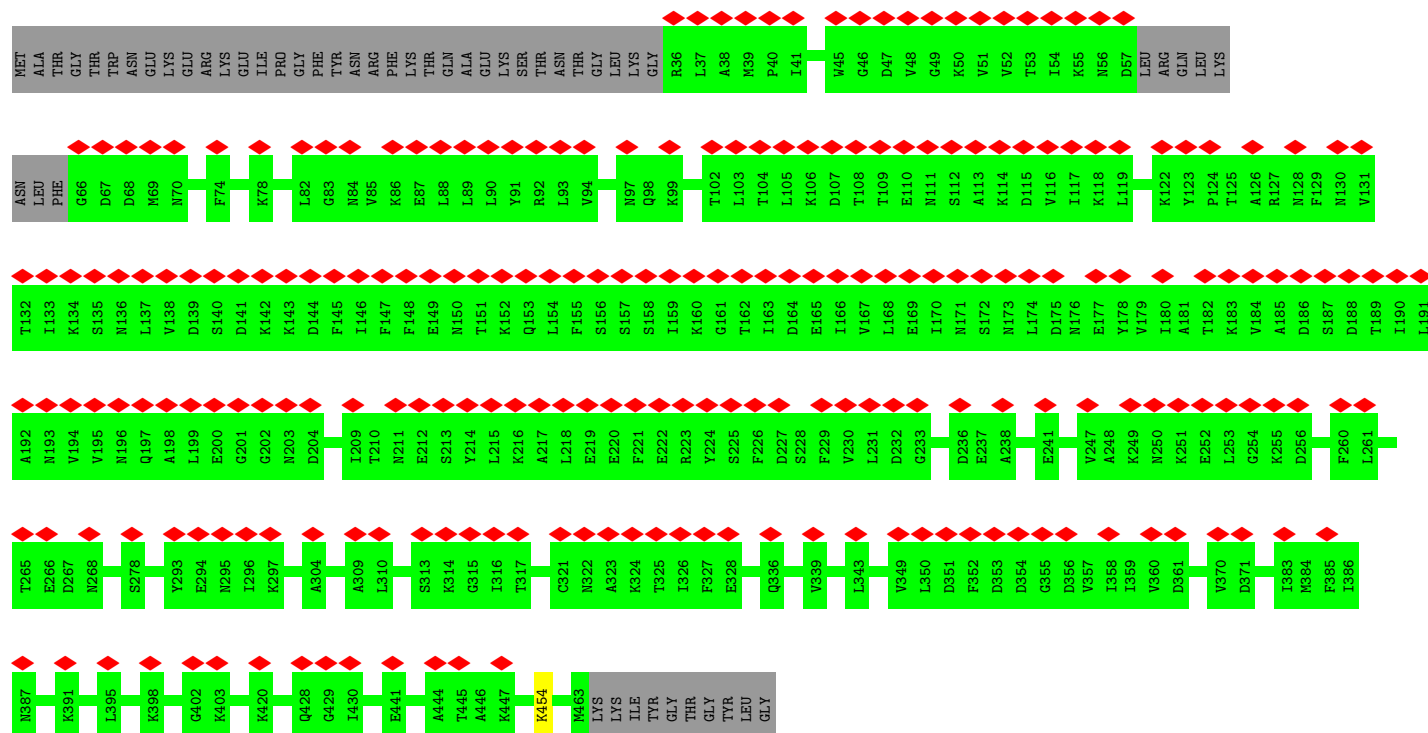
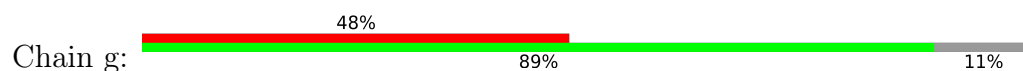


Chain f:

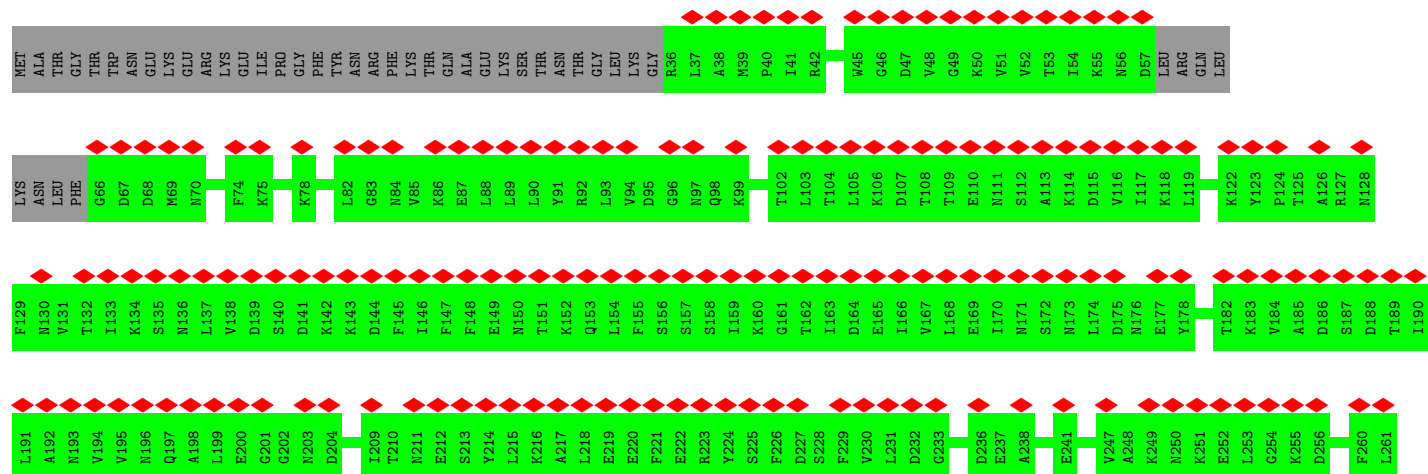
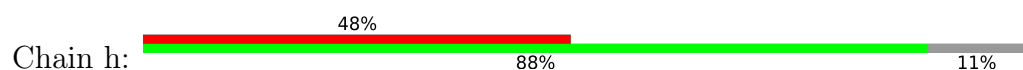


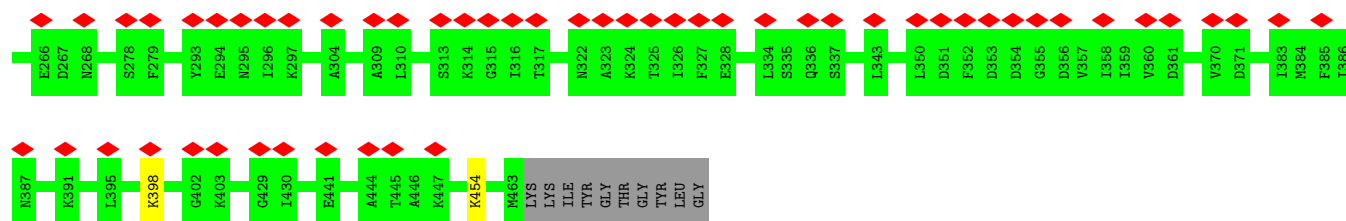


• Molecule 5: gp55 - Tail sheath protein

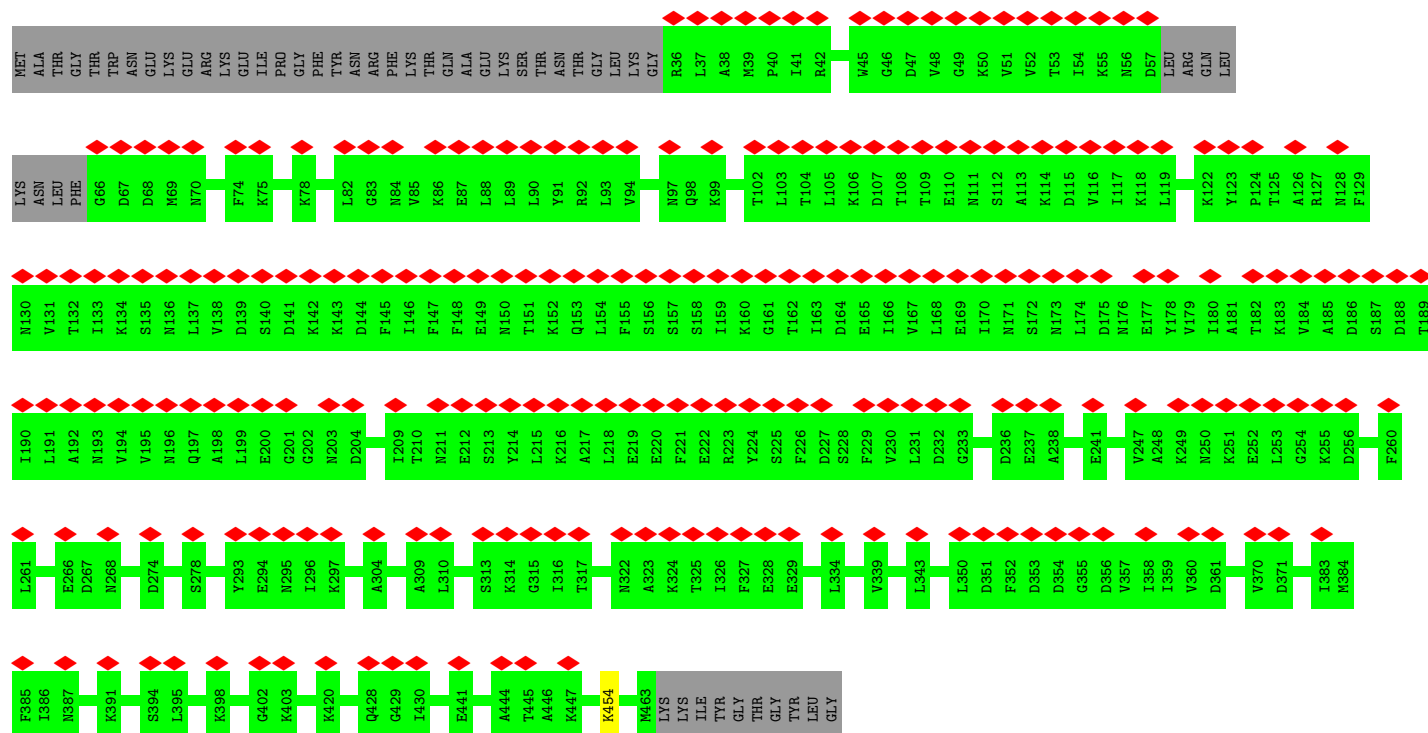
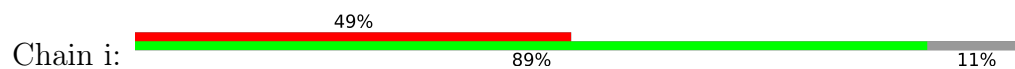


• Molecule 5: gp55 - Tail sheath protein

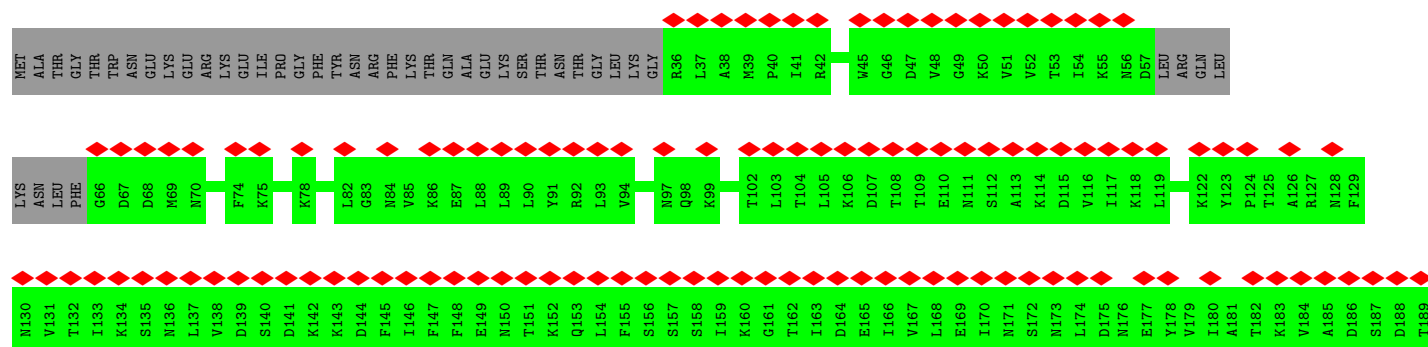
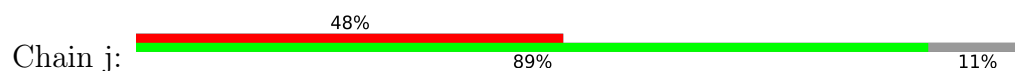


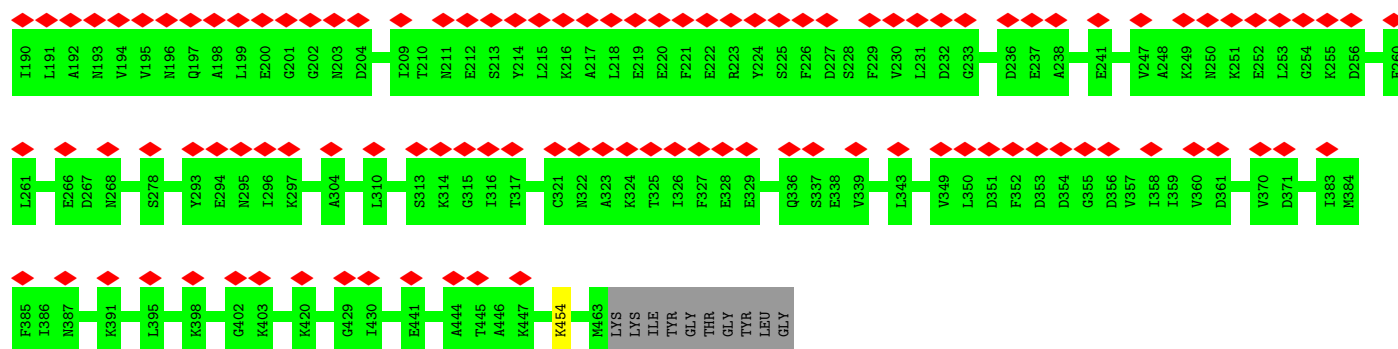


• Molecule 5: gp55 - Tail sheath protein

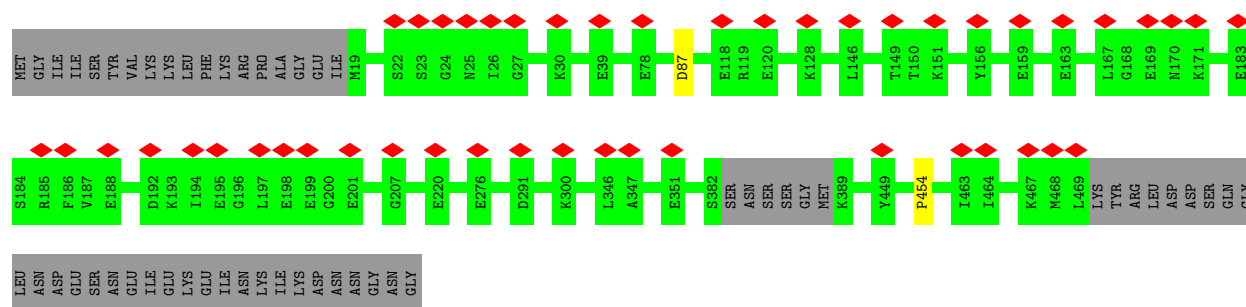


• Molecule 5: gp55 - Tail sheath protein

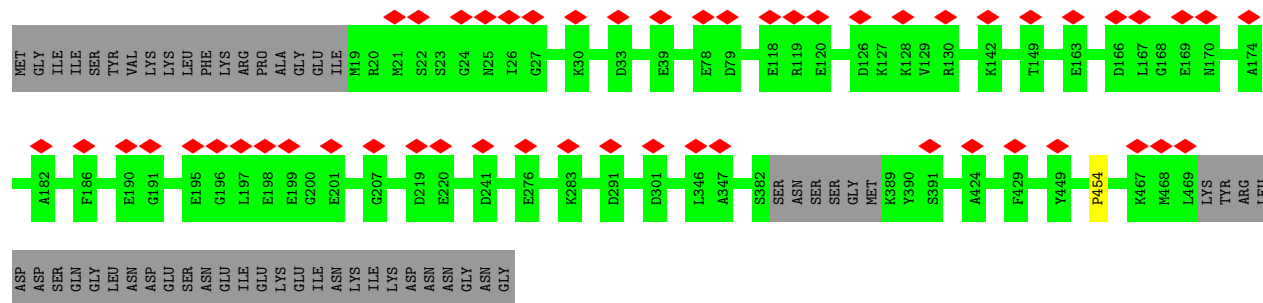
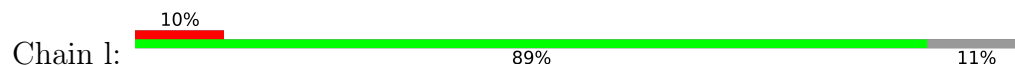




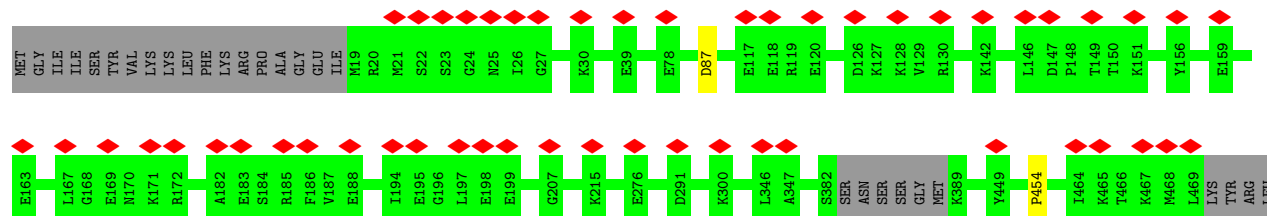
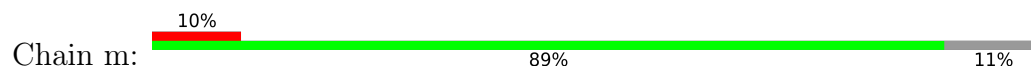
• Molecule 6: gp45 - Portal protein



• Molecule 6: gp45 - Portal protein




• Molecule 6: gp45 - Portal protein



ASP ASP
SER SER
GLN GLN
GLY GLY
LEU LEU
ASN ASN
ASP ASP
GLU GLU
SER SER
ASN ASN
GLU GLU
TLE TLE
GLU GLU
LYS LYS
TLE TLE

• Molecule 6: gp45 - Portal protein

Chain n:  9% 89% 11%

MET GLY ILE ILE SER SER TYR VAL LYS LYS LYS PHE PHE LYS ARG ARG PRO ALA ALA ILE M19 S22 S23 G24 G24 N25 I26 G27 D33 E39 E78 D79 E118 R119 E120 N121 K128 V129 R130 K142 T149 E163 D166 L167 G168 E169 N170 A174 A182 E186

E190 G191 E195 G196 L197 E198 E199 G200 E201 G207 E220 E276 E283 K283 D291 D301 L346 A347 S382 SER ASN SER SER MET K389 Y390 S391 A424 F429 Y449 P454 K467 M468 L469 LYS TYR ARG LEU ASP ASP SER GLN LEU ASN

ASP GLU SER ASN ILE GLU LYS LYS ILE ILE LYS ASP ASN GLY ASP ASN GLY

• Molecule 6: gp45 - Portal protein


Chain o:  10% 89% 11%

MET GLY ILE ILE SER SER VAL LYS LYS PHE PHE LYS ARG ARG PRO ALA ALA ILE M19 S22 S23 G24 G24 N25 I26 G27 K30 E39 E78 D87 E118 R119 E120 D126 K127 K128 V129 R130 K142 L146 D147 P148 T149 K151 Y156 E159 E163

L167 G168 E169 K171 A182 E183 S184 R185 F186 V187 E188 I194 E195 G196 L197 E198 E199 G207 K215 E220 E276 D291 K300 L346 A347 S382 SER ASN SER SER MET K389 Y449 P454 L463 L464 K467 M468 L469 LYS TYR ARG ASP

ASP SER GLN GLY LEU ASN ASP GLU SER SER ASN GLU ILE ILE LYS GLU ASN ILE ILE ASP ASN GLY ASP ASN GLY

• Molecule 6: gp45 - Portal protein


Chain p:  10% 89% 11%

MET GLY ILE ILE SER SER VAL LYS LYS PHE PHE LYS ARG ARG PRO ALA ALA ILE M19 S22 S23 G24 G24 N25 I26 G27 D33 E39 E78 D79 E118 R119 E120 D126 K127 K128 V129 R130 K142 T149 E163 D166 L167 G168 E169 N170 A174 A182

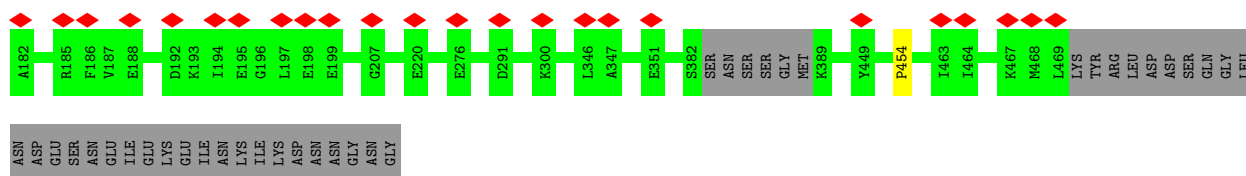
F186 E190 G191 E195 G196 L197 E198 E199 G200 E201 G207 E220 E276 K283 D291 D301 L346 A347 S382 SER ASN SER SER MET K389 Y390 S391 A424 F429 Y449 P454 K467 M468 L469 LYS TYR ARG LEU ASP ASP SER GLN LEU

ASN ASP GLU SER ASN GLU ILE GLU LYS LYS PHE PHE ILE ILE LYS ASP ASN GLY ASN ASN GLY

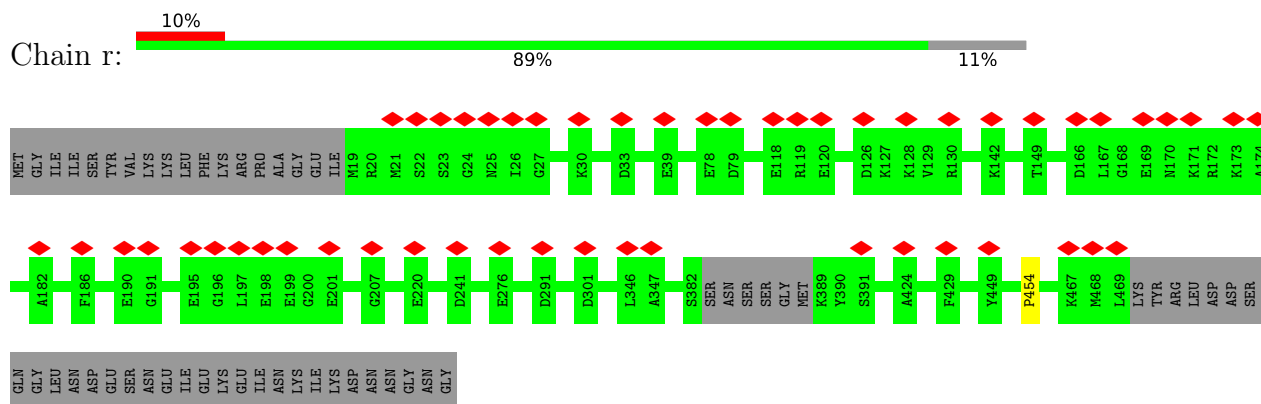
• Molecule 6: gp45 - Portal protein

Chain q:  9% 89% 11%

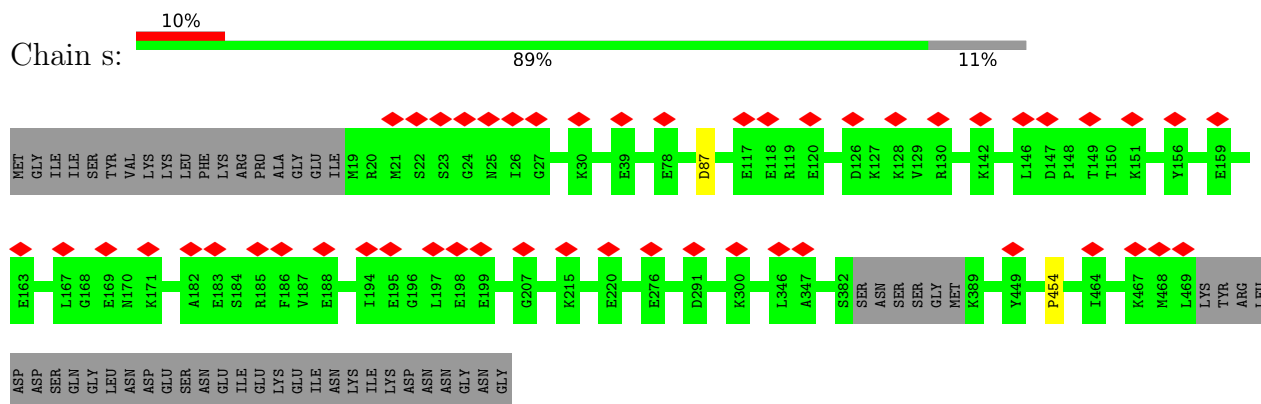
MET GLY ILE ILE SER SER VAL LYS LYS PHE PHE LYS ARG ARG PRO ALA ALA ILE M19 R20 M21 S22 S23 G24 G24 N25 I26 G27 K30 E39 E78 D87 E118 R119 E120 K128 L146 T149 T150 K151 Y156 E159 E163 L167 G168 E169 M170 K171



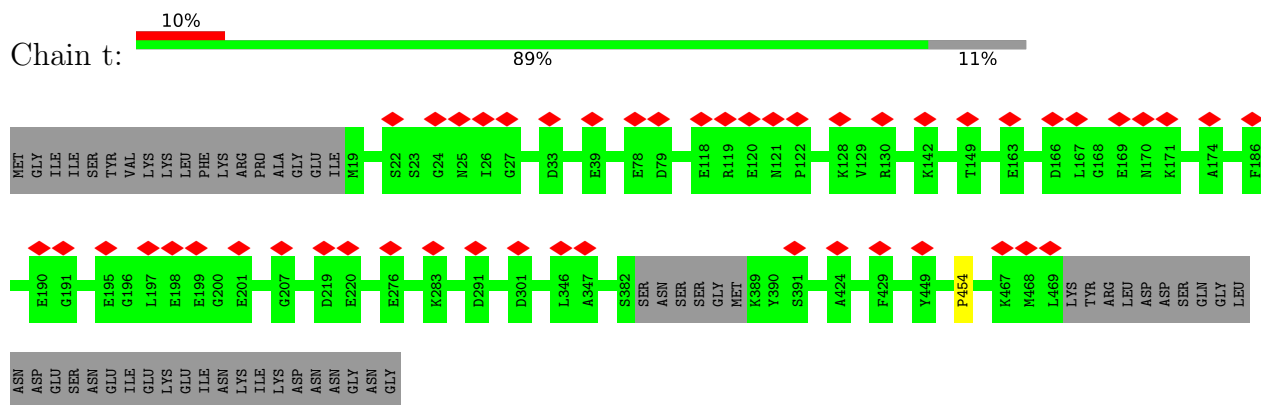
• Molecule 6: gp45 - Portal protein



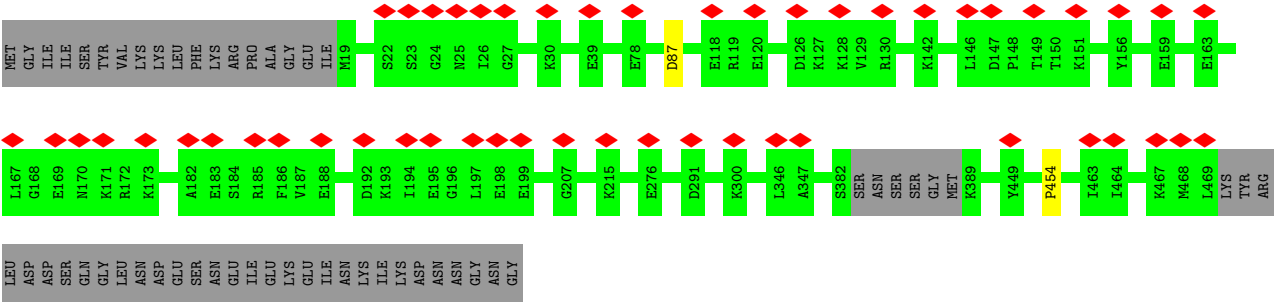
• Molecule 6: gp45 - Portal protein



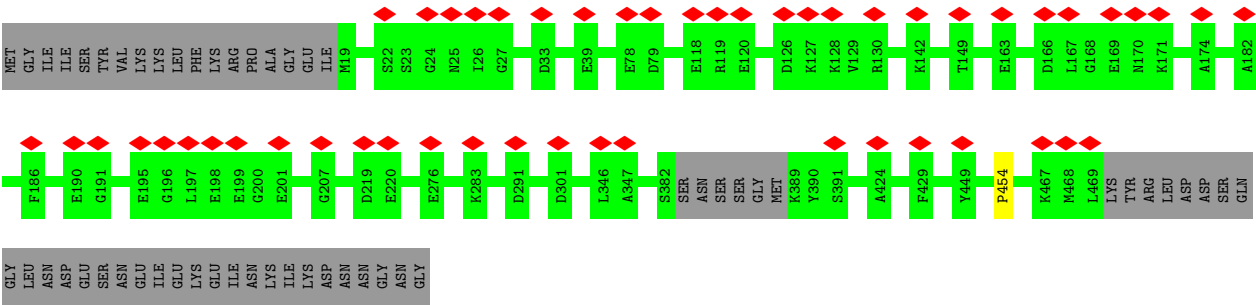
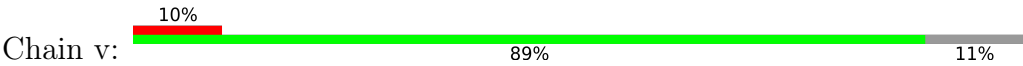
• Molecule 6: gp45 - Portal protein



• Molecule 6: gp45 - Portal protein



● Molecule 6: gp45 - Portal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23724	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.587	Depositor
Minimum map value	-0.751	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.27	0/1041	0.56	0/1394
1	B	0.27	0/1041	0.56	0/1394
1	C	0.27	0/1041	0.56	0/1394
1	D	0.27	0/1041	0.55	0/1394
1	E	0.27	0/1041	0.56	0/1394
1	F	0.27	0/1041	0.56	0/1394
2	G	0.27	0/1007	0.59	0/1353
2	K	0.27	0/1007	0.59	0/1353
2	M	0.27	0/1007	0.59	0/1353
2	O	0.27	0/1007	0.59	0/1353
2	Q	0.27	0/1007	0.58	0/1353
2	X	0.27	0/1007	0.59	0/1353
3	H	0.27	0/2249	0.56	0/3030
3	L	0.27	0/2249	0.55	0/3030
3	N	0.27	0/2249	0.55	0/3030
3	P	0.27	0/2249	0.55	0/3030
3	R	0.27	0/2249	0.56	0/3030
3	d	0.27	0/2249	0.55	0/3030
4	I	0.29	0/845	0.46	0/1130
4	J	0.30	0/845	0.48	0/1130
4	S	0.30	0/845	0.47	0/1130
4	T	0.29	0/845	0.45	0/1130
4	U	0.30	0/845	0.45	0/1130
4	V	0.30	0/845	0.47	0/1130
4	W	0.29	0/845	0.46	0/1130
4	Y	0.29	0/845	0.46	0/1130
4	Z	0.30	0/845	0.46	0/1130
4	a	0.29	0/845	0.47	0/1130
4	b	0.29	0/845	0.47	0/1130
4	c	0.29	0/845	0.47	0/1130
5	e	0.26	0/3340	0.48	0/4508
5	f	0.26	0/3340	0.48	0/4508
5	g	0.26	0/3340	0.48	0/4508
5	h	0.26	0/3340	0.48	0/4508

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	i	0.26	0/3340	0.48	0/4508
5	j	0.26	0/3340	0.48	0/4508
6	k	0.27	0/3566	0.50	1/4820 (0.0%)
6	l	0.27	0/3566	0.51	0/4820
6	m	0.27	0/3566	0.51	1/4820 (0.0%)
6	n	0.27	0/3566	0.50	0/4820
6	o	0.27	0/3566	0.50	1/4820 (0.0%)
6	p	0.27	0/3566	0.51	0/4820
6	q	0.27	0/3566	0.51	1/4820 (0.0%)
6	r	0.27	0/3566	0.50	0/4820
6	s	0.27	0/3566	0.50	1/4820 (0.0%)
6	t	0.27	0/3566	0.51	0/4820
6	u	0.27	0/3566	0.51	1/4820 (0.0%)
6	v	0.27	0/3566	0.51	0/4820
All	All	0.27	0/98754	0.51	6/133110 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	q	87	ASP	CB-CG-OD1	5.39	123.15	118.30
6	o	87	ASP	CB-CG-OD1	5.39	123.15	118.30
6	k	87	ASP	CB-CG-OD1	5.38	123.15	118.30
6	s	87	ASP	CB-CG-OD1	5.37	123.13	118.30
6	m	87	ASP	CB-CG-OD1	5.34	123.11	118.30

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	1029	1031	1030	7	0
1	B	1029	1031	1030	7	0
1	C	1029	1031	1030	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1029	1031	1030	12	0
1	E	1029	1031	1030	10	0
1	F	1029	1031	1030	8	0
2	G	998	1021	1020	7	0
2	K	998	1021	1020	9	0
2	M	998	1021	1020	9	0
2	O	998	1021	1020	10	0
2	Q	998	1021	1020	9	0
2	X	998	1021	1020	10	0
3	H	2215	2247	2244	23	0
3	L	2215	2247	2244	22	0
3	N	2215	2247	2244	19	0
3	P	2215	2247	2244	21	0
3	R	2215	2247	2244	22	0
3	d	2215	2247	2244	0	0
4	I	833	816	815	6	0
4	J	833	816	815	5	0
4	S	833	816	815	7	0
4	T	833	816	815	8	0
4	U	833	816	815	6	0
4	V	833	816	815	4	0
4	W	833	816	815	4	0
4	Y	833	816	815	4	0
4	Z	833	816	815	3	0
4	a	833	816	815	0	0
4	b	833	816	815	0	0
4	c	833	816	815	0	0
5	e	3296	3289	3287	0	0
5	f	3296	3289	3287	0	0
5	g	3296	3289	3287	0	0
5	h	3296	3289	3287	0	0
5	i	3296	3289	3287	0	0
5	j	3296	3289	3287	0	0
6	k	3497	3429	3421	0	0
6	l	3497	3429	3421	0	0
6	m	3497	3429	3421	0	0
6	n	3497	3429	3421	0	0
6	o	3497	3429	3421	0	0
6	p	3497	3429	3421	0	0
6	q	3497	3429	3421	0	0
6	r	3497	3429	3421	0	0
6	s	3497	3429	3421	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	t	3497	3429	3421	0	0
6	u	3497	3429	3421	0	0
6	v	3497	3429	3421	0	0
All	All	97188	96468	96318	212	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 4.

The worst 5 of 212 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)
3:H:104:ASP:OD2	3:N:2:ARG:NH2	2.14	0.80
3:P:104:ASP:OD2	3:R:2:ARG:NH2	2.15	0.80
3:H:2:ARG:NH2	3:L:104:ASP:OD2	2.15	0.79
3:N:104:ASP:OD2	3:P:2:ARG:NH2	2.15	0.78
4:J:85:ASN:OD1	4:S:83:TYR:OH	2.05	0.73

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	128/137 (93%)	123 (96%)	5 (4%)	0	100	100
1	B	128/137 (93%)	123 (96%)	5 (4%)	0	100	100
1	C	128/137 (93%)	124 (97%)	4 (3%)	0	100	100
1	D	128/137 (93%)	124 (97%)	4 (3%)	0	100	100
1	E	128/137 (93%)	124 (97%)	4 (3%)	0	100	100
1	F	128/137 (93%)	125 (98%)	3 (2%)	0	100	100
2	G	122/125 (98%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	M	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	O	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	Q	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
2	X	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
3	H	270/273 (99%)	260 (96%)	10 (4%)	0	100	100
3	L	270/273 (99%)	261 (97%)	9 (3%)	0	100	100
3	N	270/273 (99%)	260 (96%)	10 (4%)	0	100	100
3	P	270/273 (99%)	261 (97%)	9 (3%)	0	100	100
3	R	270/273 (99%)	261 (97%)	9 (3%)	0	100	100
3	d	270/273 (99%)	260 (96%)	10 (4%)	0	100	100
4	I	101/112 (90%)	100 (99%)	1 (1%)	0	100	100
4	J	101/112 (90%)	100 (99%)	1 (1%)	0	100	100
4	S	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
4	T	101/112 (90%)	100 (99%)	1 (1%)	0	100	100
4	U	101/112 (90%)	96 (95%)	5 (5%)	0	100	100
4	V	101/112 (90%)	97 (96%)	4 (4%)	0	100	100
4	W	101/112 (90%)	100 (99%)	1 (1%)	0	100	100
4	Y	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
4	Z	101/112 (90%)	98 (97%)	3 (3%)	0	100	100
4	a	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
4	b	101/112 (90%)	100 (99%)	1 (1%)	0	100	100
4	c	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
5	e	416/473 (88%)	393 (94%)	23 (6%)	0	100	100
5	f	416/473 (88%)	394 (95%)	22 (5%)	0	100	100
5	g	416/473 (88%)	392 (94%)	24 (6%)	0	100	100
5	h	416/473 (88%)	394 (95%)	22 (5%)	0	100	100
5	i	416/473 (88%)	394 (95%)	22 (5%)	0	100	100
5	j	416/473 (88%)	396 (95%)	20 (5%)	0	100	100
6	k	441/500 (88%)	433 (98%)	7 (2%)	1 (0%)	44	72
6	l	441/500 (88%)	434 (98%)	6 (1%)	1 (0%)	44	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	m	441/500 (88%)	434 (98%)	6 (1%)	1 (0%)	44	72
6	n	441/500 (88%)	433 (98%)	7 (2%)	1 (0%)	44	72
6	o	441/500 (88%)	434 (98%)	6 (1%)	1 (0%)	44	72
6	p	441/500 (88%)	433 (98%)	7 (2%)	1 (0%)	44	72
6	q	441/500 (88%)	434 (98%)	6 (1%)	1 (0%)	44	72
6	r	441/500 (88%)	434 (98%)	6 (1%)	1 (0%)	44	72
6	s	441/500 (88%)	434 (98%)	6 (1%)	1 (0%)	44	72
6	t	441/500 (88%)	434 (98%)	6 (1%)	1 (0%)	44	72
6	u	441/500 (88%)	433 (98%)	7 (2%)	1 (0%)	44	72
6	v	441/500 (88%)	432 (98%)	8 (2%)	1 (0%)	44	72
All	All	12120/13392 (90%)	11772 (97%)	336 (3%)	12 (0%)	50	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	k	454	PRO
6	l	454	PRO
6	m	454	PRO
6	n	454	PRO
6	o	454	PRO

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	A	115/122 (94%)	115 (100%)	0	100	100
1	B	115/122 (94%)	115 (100%)	0	100	100
1	C	115/122 (94%)	115 (100%)	0	100	100
1	D	115/122 (94%)	115 (100%)	0	100	100
1	E	115/122 (94%)	115 (100%)	0	100	100
1	F	115/122 (94%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	116/117 (99%)	116 (100%)	0	100	100
2	K	116/117 (99%)	116 (100%)	0	100	100
2	M	116/117 (99%)	116 (100%)	0	100	100
2	O	116/117 (99%)	116 (100%)	0	100	100
2	Q	116/117 (99%)	116 (100%)	0	100	100
2	X	116/117 (99%)	116 (100%)	0	100	100
3	H	249/250 (100%)	249 (100%)	0	100	100
3	L	249/250 (100%)	249 (100%)	0	100	100
3	N	249/250 (100%)	249 (100%)	0	100	100
3	P	249/250 (100%)	249 (100%)	0	100	100
3	R	249/250 (100%)	249 (100%)	0	100	100
3	d	249/250 (100%)	249 (100%)	0	100	100
4	I	93/101 (92%)	93 (100%)	0	100	100
4	J	93/101 (92%)	93 (100%)	0	100	100
4	S	93/101 (92%)	93 (100%)	0	100	100
4	T	93/101 (92%)	93 (100%)	0	100	100
4	U	93/101 (92%)	93 (100%)	0	100	100
4	V	93/101 (92%)	93 (100%)	0	100	100
4	W	93/101 (92%)	93 (100%)	0	100	100
4	Y	93/101 (92%)	93 (100%)	0	100	100
4	Z	93/101 (92%)	93 (100%)	0	100	100
4	a	93/101 (92%)	93 (100%)	0	100	100
4	b	93/101 (92%)	93 (100%)	0	100	100
4	c	93/101 (92%)	93 (100%)	0	100	100
5	e	369/413 (89%)	368 (100%)	1 (0%)	91	95
5	f	369/413 (89%)	368 (100%)	1 (0%)	91	95
5	g	369/413 (89%)	368 (100%)	1 (0%)	91	95
5	h	369/413 (89%)	367 (100%)	2 (0%)	86	91
5	i	369/413 (89%)	368 (100%)	1 (0%)	91	95
5	j	369/413 (89%)	368 (100%)	1 (0%)	91	95
6	k	374/448 (84%)	374 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	l	374/448 (84%)	374 (100%)	0	100	100
6	m	374/448 (84%)	374 (100%)	0	100	100
6	n	374/448 (84%)	374 (100%)	0	100	100
6	o	374/448 (84%)	374 (100%)	0	100	100
6	p	374/448 (84%)	374 (100%)	0	100	100
6	q	374/448 (84%)	374 (100%)	0	100	100
6	r	374/448 (84%)	374 (100%)	0	100	100
6	s	374/448 (84%)	374 (100%)	0	100	100
6	t	374/448 (84%)	374 (100%)	0	100	100
6	u	374/448 (84%)	374 (100%)	0	100	100
6	v	374/448 (84%)	374 (100%)	0	100	100
All	All	10698/12000 (89%)	10691 (100%)	7 (0%)	92	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	h	398	LYS
5	h	454	LYS
5	j	454	LYS
5	i	454	LYS
5	g	454	LYS

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.

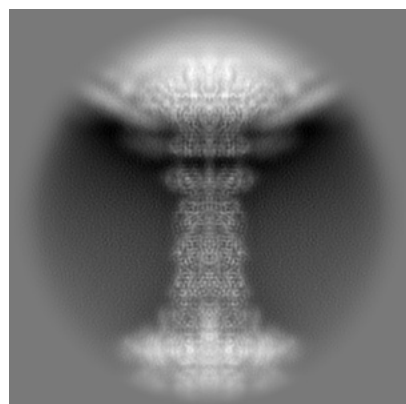
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51200. These allow visual inspection of the internal detail of the map and identification of artifacts.

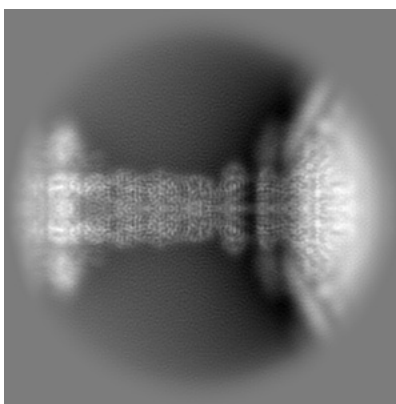
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

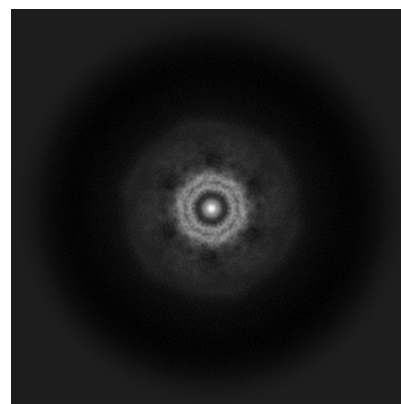
6.1.1 Primary map



X

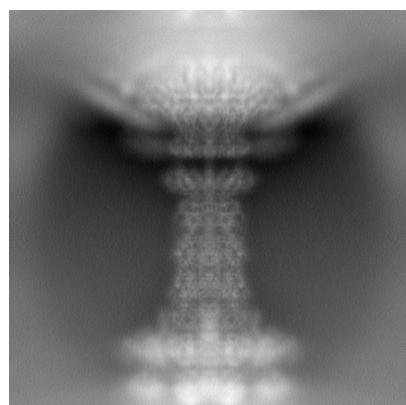


Y

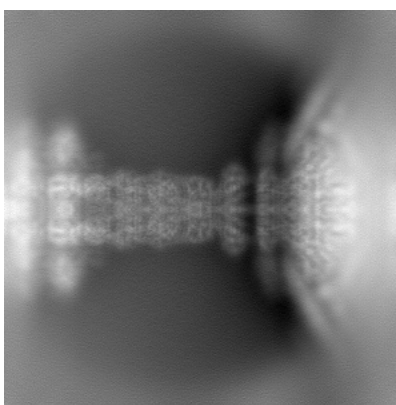


Z

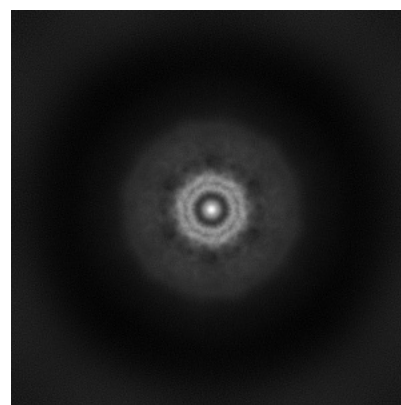
6.1.2 Raw map



X



Y

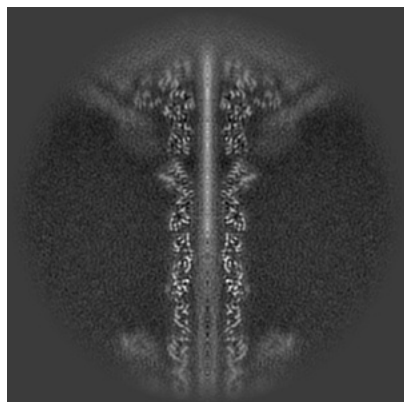


Z

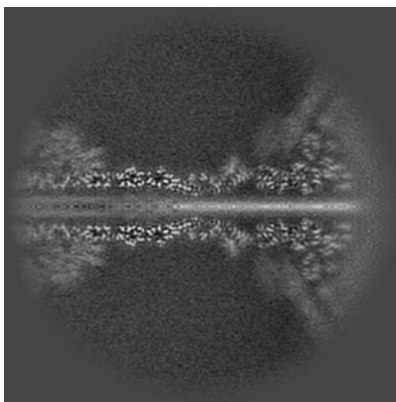
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

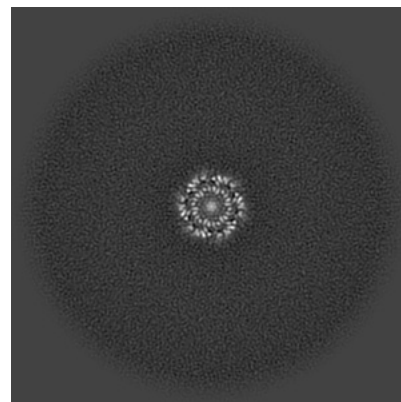
6.2.1 Primary map



X Index: 200

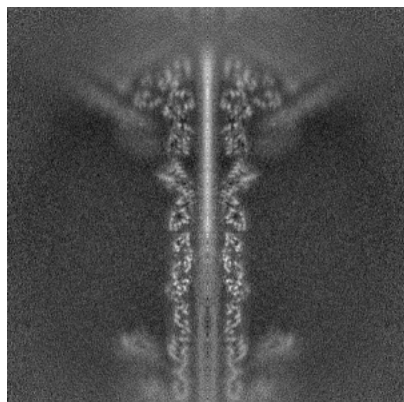


Y Index: 200

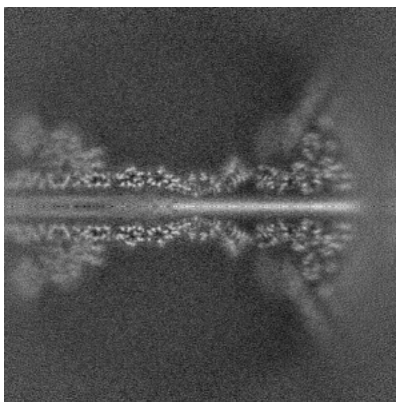


Z Index: 200

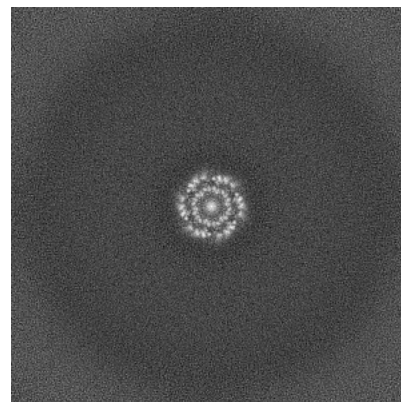
6.2.2 Raw map



X Index: 200



Y Index: 200

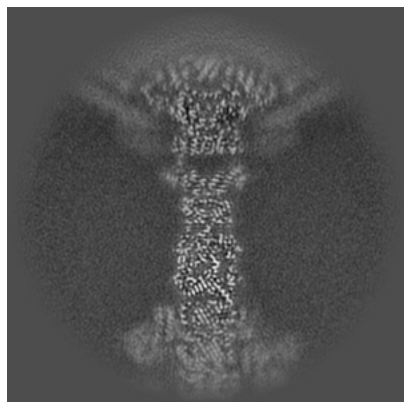


Z Index: 200

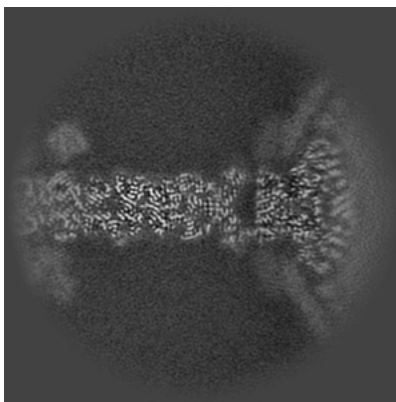
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

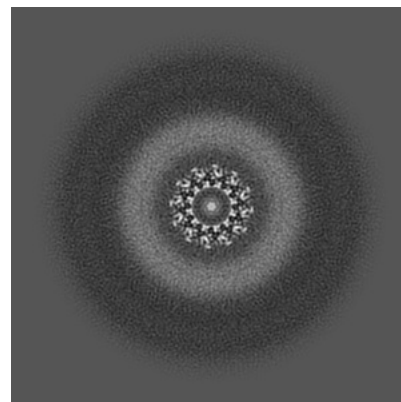
6.3.1 Primary map



X Index: 180

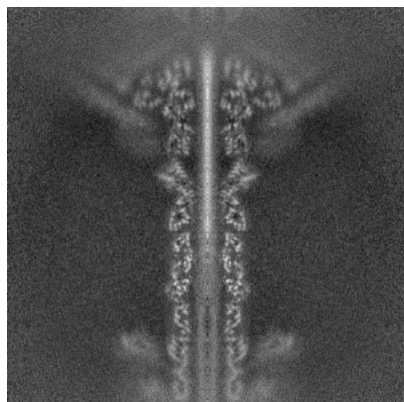


Y Index: 219

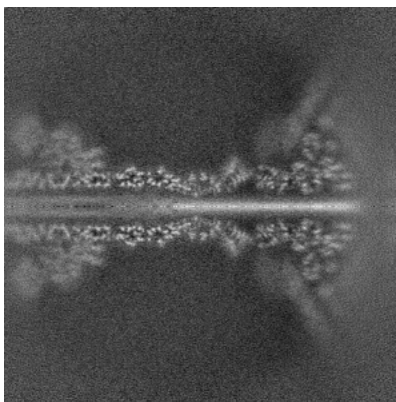


Z Index: 287

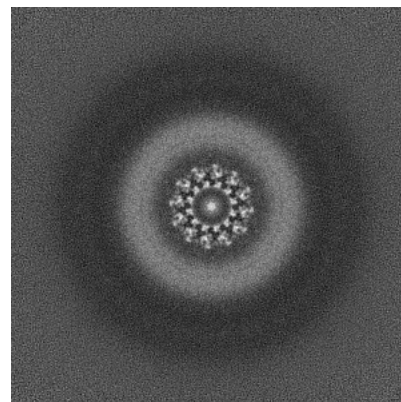
6.3.2 Raw map



X Index: 200



Y Index: 200

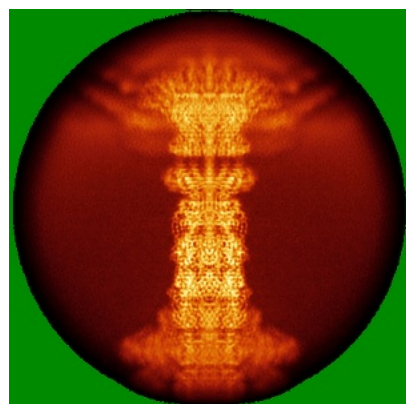


Z Index: 287

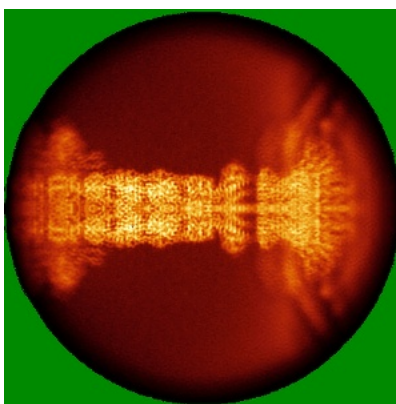
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

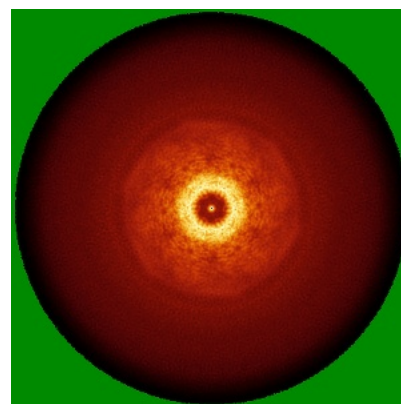
6.4.1 Primary map



X

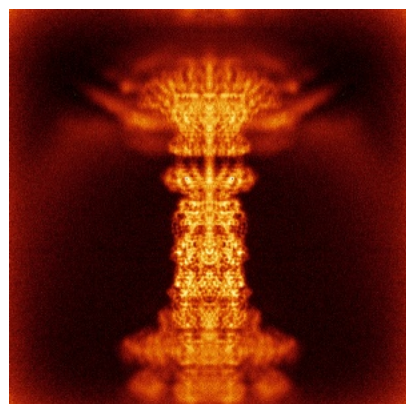


Y

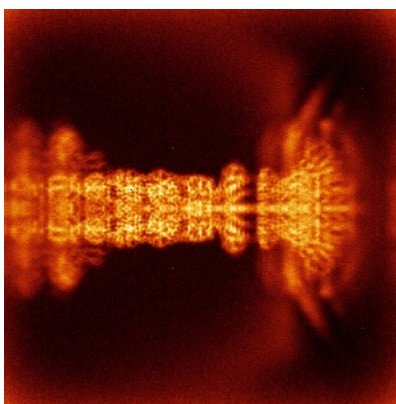


Z

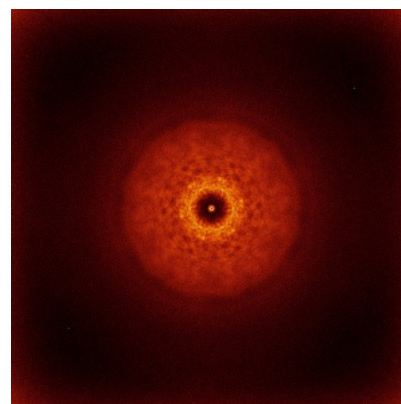
6.4.2 Raw map



X



Y

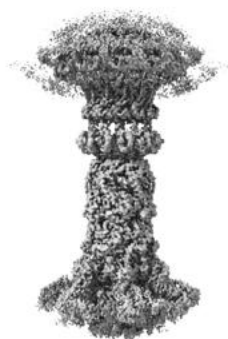


Z

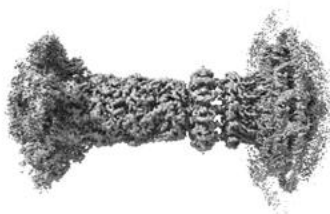
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

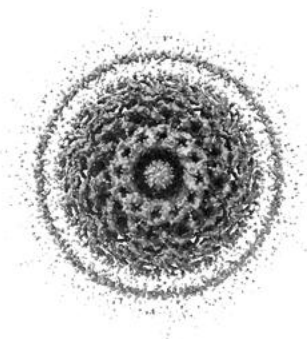
6.5.1 Primary map



X



Y



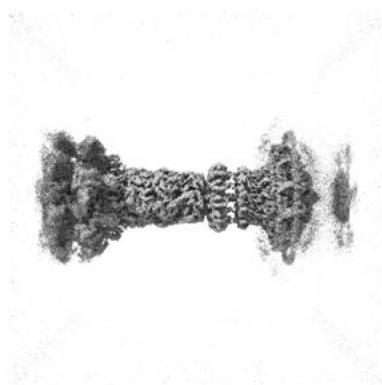
Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

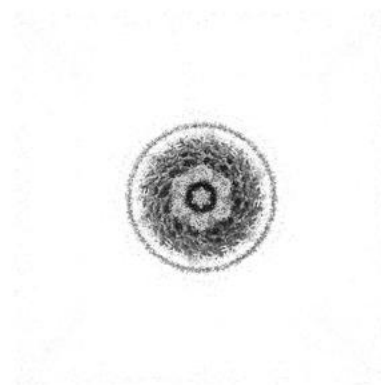
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

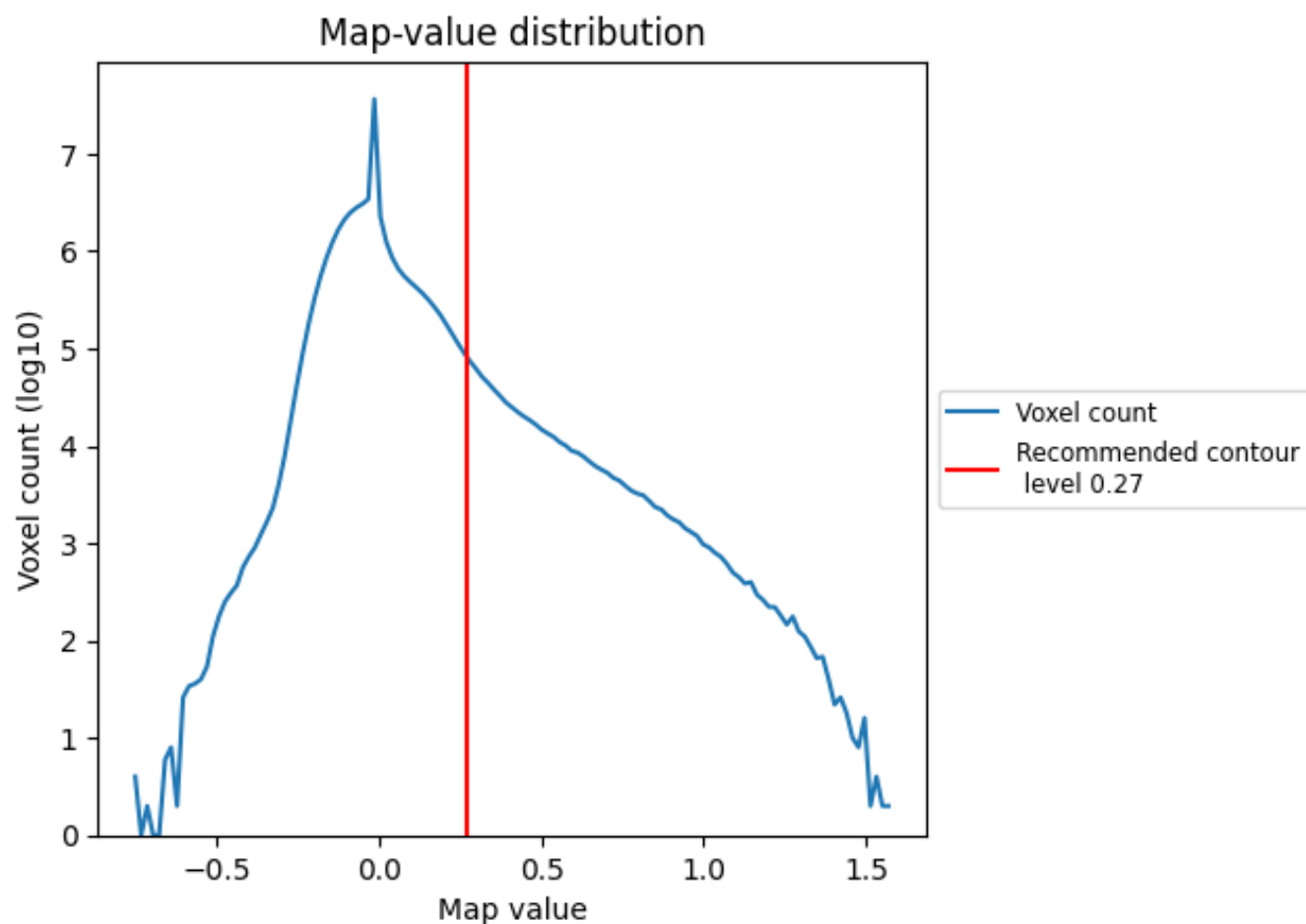
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

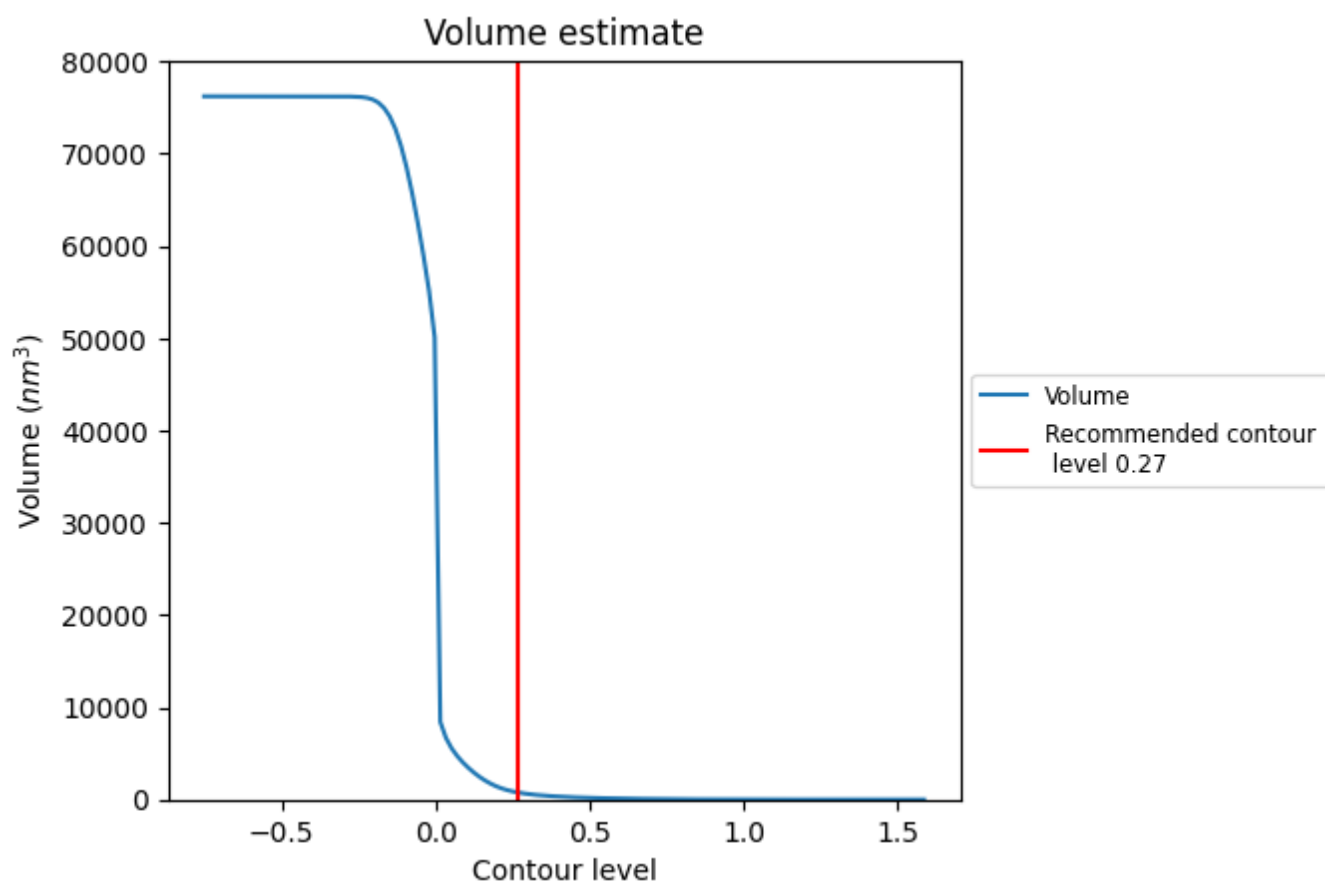
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

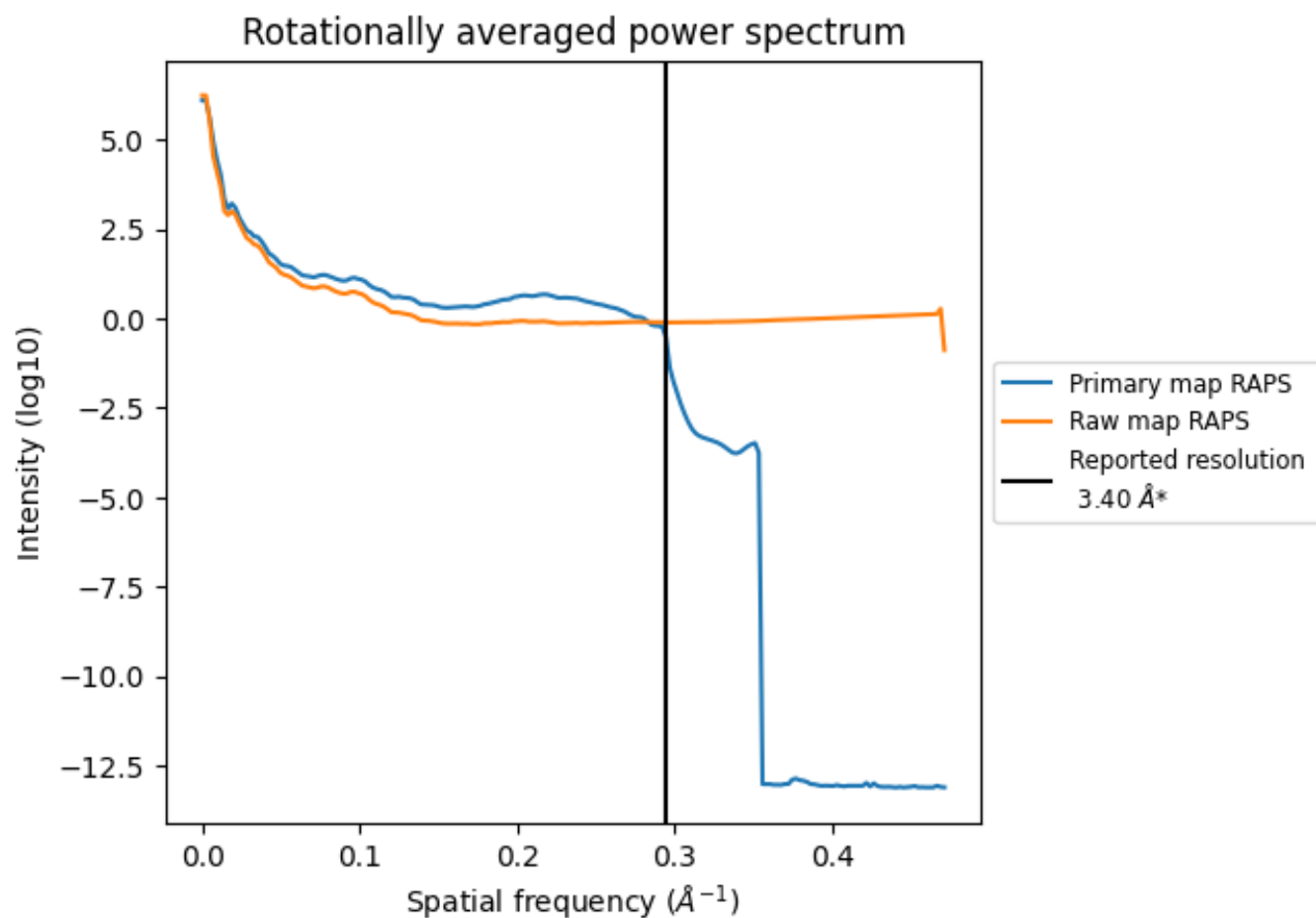
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 759 nm³; this corresponds to an approximate mass of 685 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 ⓘ

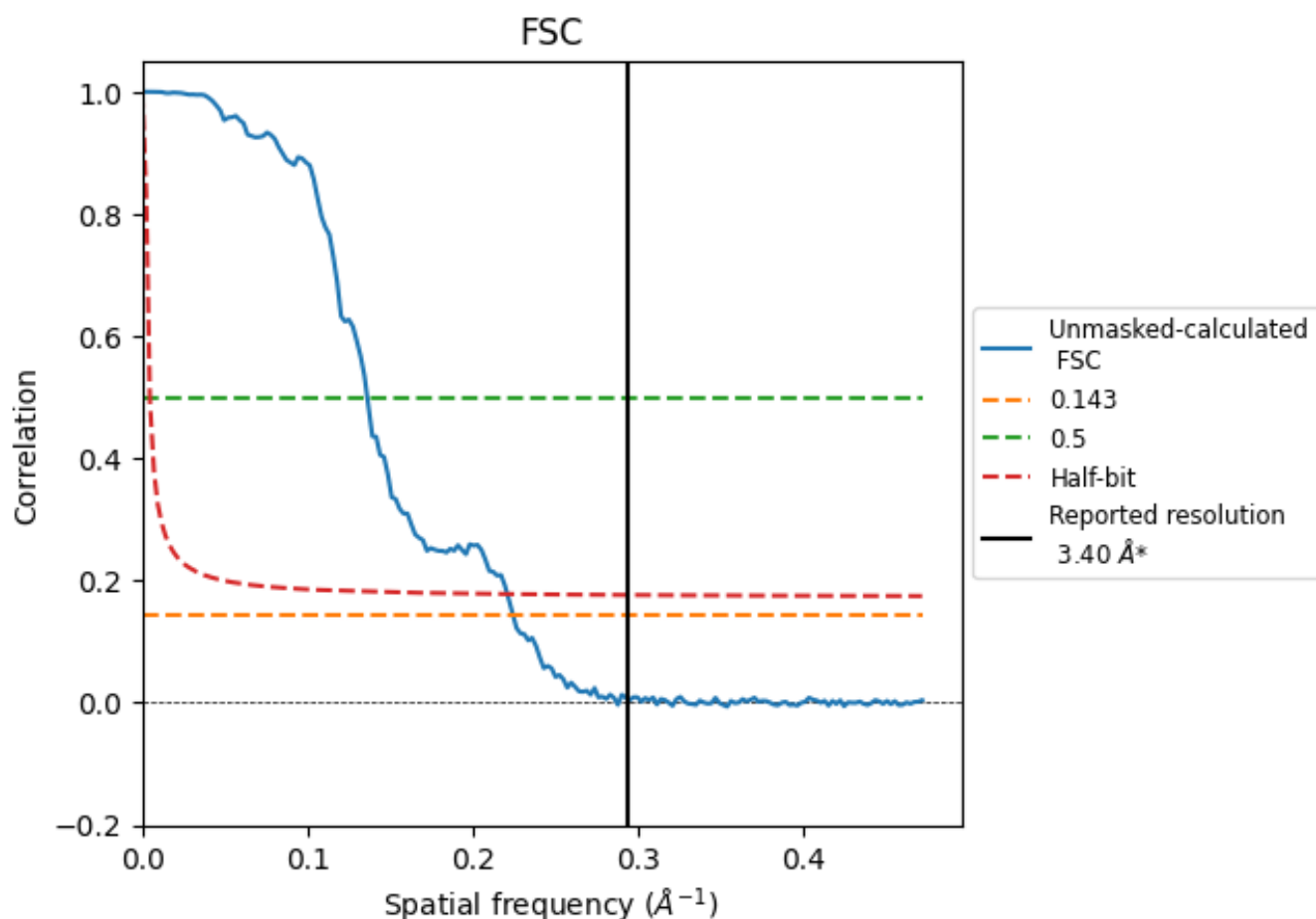


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

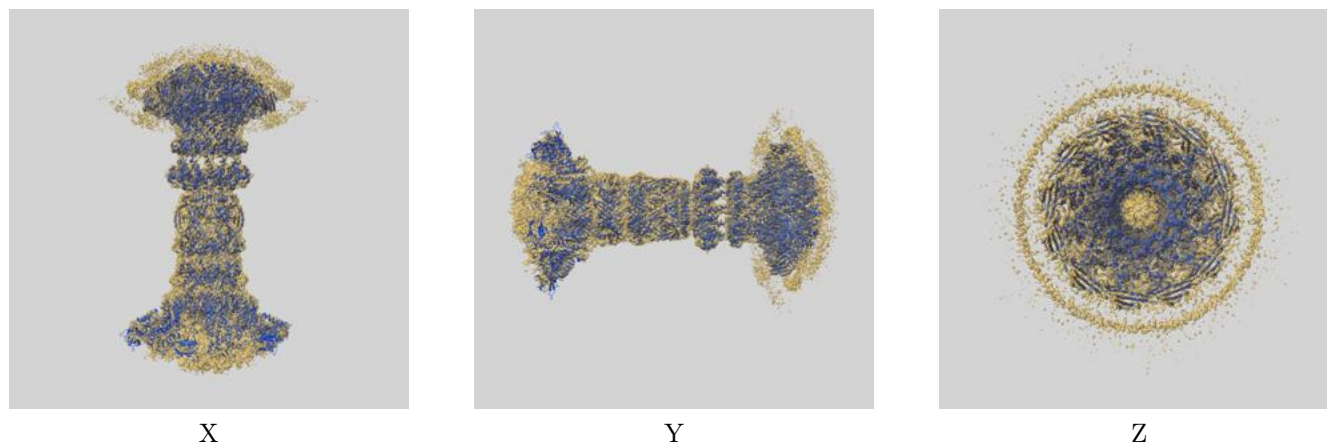
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.46	7.35	4.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.46 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

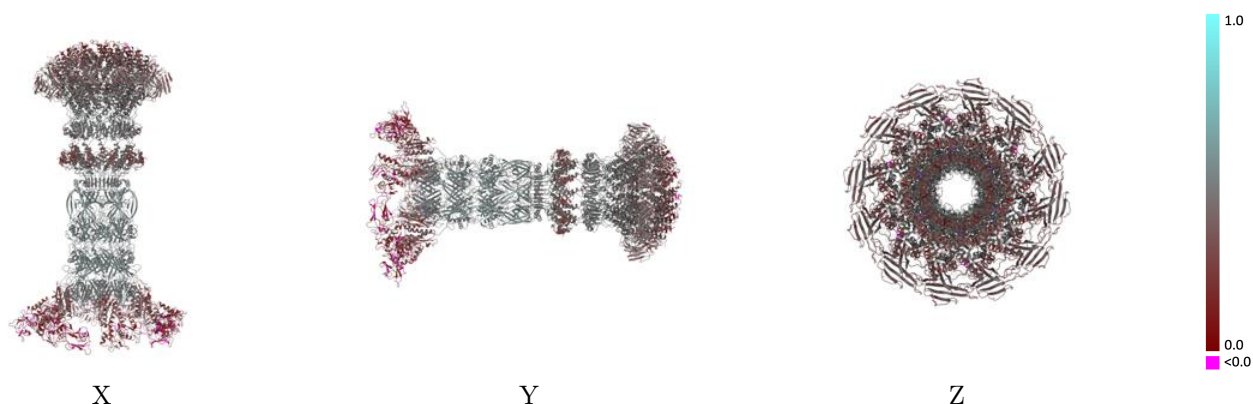
This section contains information regarding the fit between EMDB map EMD-51200 and PDB model 9GB7. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



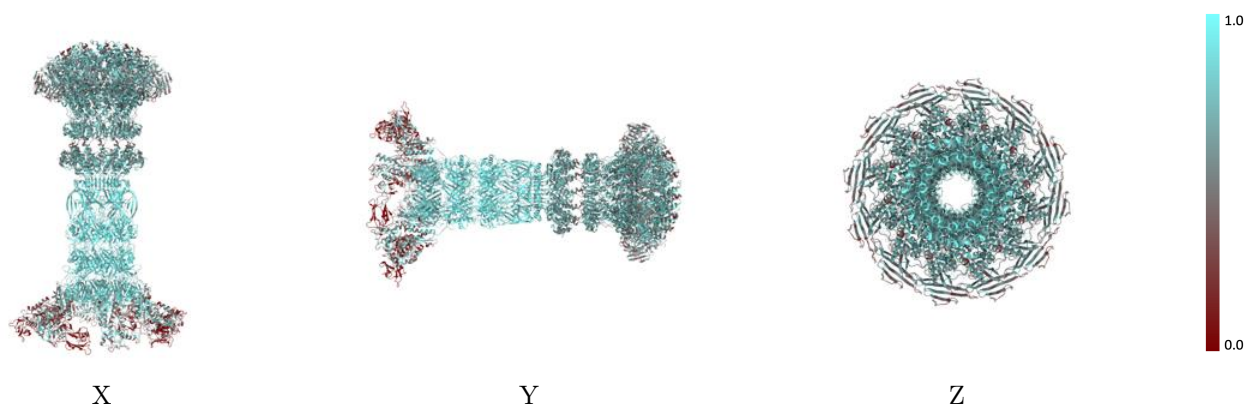
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



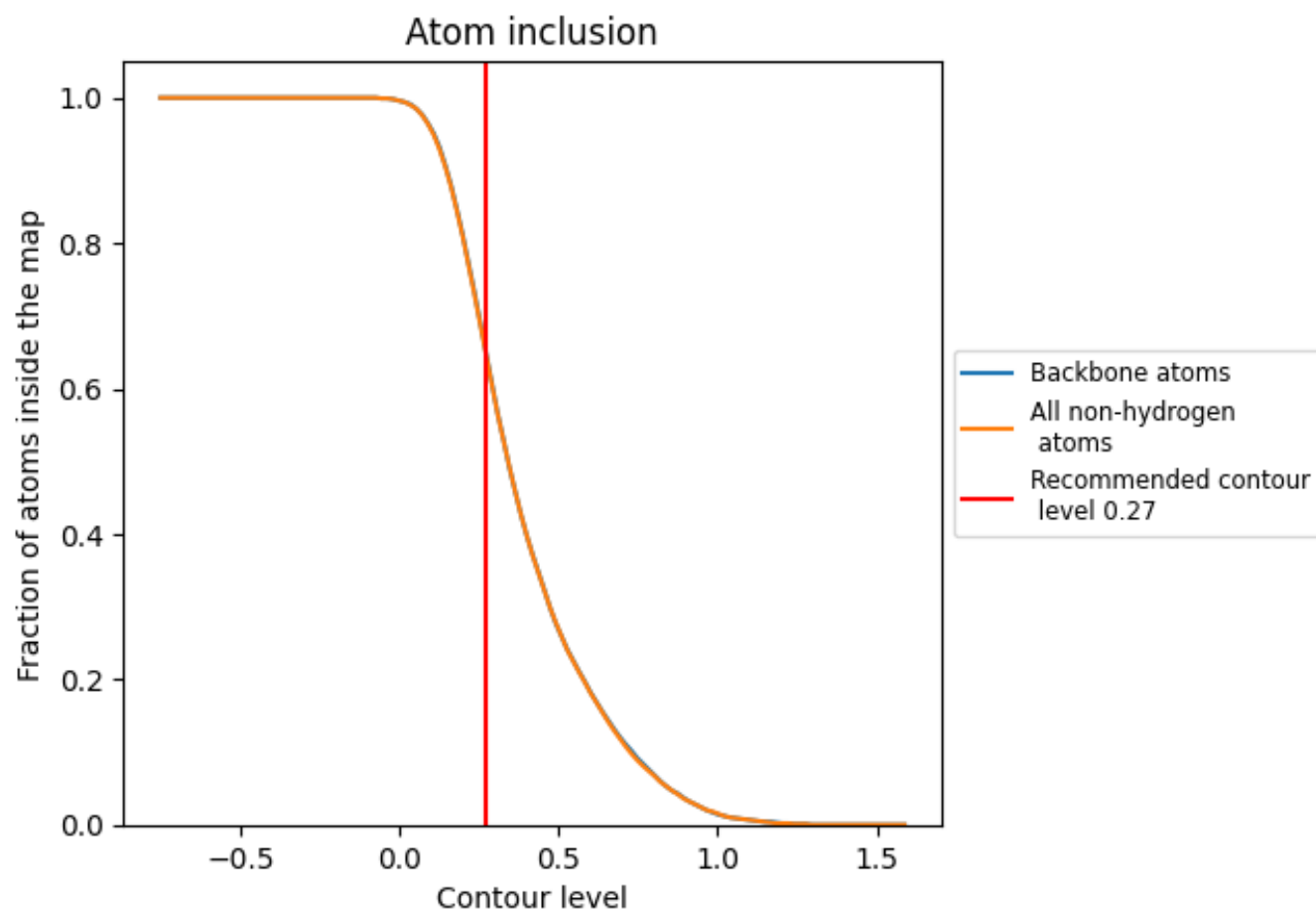
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.27).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6510	 0.3960
A	 0.8380	 0.5010
B	 0.8450	 0.5030
C	 0.8370	 0.5010
D	 0.8400	 0.5010
E	 0.8460	 0.5010
F	 0.8400	 0.5000
G	 0.8750	 0.5060
H	 0.8730	 0.5070
I	 0.6950	 0.4330
J	 0.6640	 0.4080
K	 0.8700	 0.5050
L	 0.8770	 0.5070
M	 0.8710	 0.5070
N	 0.8780	 0.5060
O	 0.8750	 0.5060
P	 0.8770	 0.5070
Q	 0.8690	 0.5030
R	 0.8730	 0.5090
S	 0.7040	 0.4300
T	 0.6980	 0.4390
U	 0.7000	 0.4370
V	 0.7020	 0.4330
W	 0.7090	 0.4380
X	 0.8740	 0.5040
Y	 0.6700	 0.4150
Z	 0.6710	 0.4130
a	 0.6610	 0.4150
b	 0.6650	 0.4150
c	 0.6750	 0.4190
d	 0.8770	 0.5080
e	 0.3740	 0.2240
f	 0.3750	 0.2220
g	 0.3740	 0.2220
h	 0.3730	 0.2220



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Chain	Atom inclusion	Q-score
i	 0.3710	 0.2210
j	 0.3740	 0.2200
k	 0.6630	 0.4130
l	 0.6530	 0.3970
m	 0.6580	 0.4130
n	 0.6540	 0.3960
o	 0.6590	 0.4130
p	 0.6530	 0.3960
q	 0.6640	 0.4130
r	 0.6550	 0.3980
s	 0.6600	 0.4110
t	 0.6530	 0.3970
u	 0.6590	 0.4130
v	 0.6510	 0.3960