



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2024 – 07:22 PM JST

PDB ID : 8Y6V
EMDB ID : EMD-39002
Title : Near-atomic structure of icosahedrally averaged jumbo bacteriophage PhiKZ capsid
Authors : Yang, Y.; Shao, Q.; Guo, M.; Han, L.; Zhao, X.; Wang, A.; Li, X.; Wang, B.; Pan, J.; Chen, Z.; Fokine, A.; Sun, L.; Fang, Q.
Deposited on : 2024-02-03
Resolution : 3.50 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:

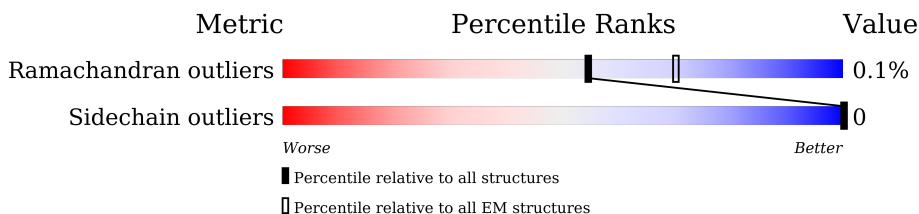
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.50 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	D	320	
2	B	271	
3	E	149	
3	F	149	
4	G	428	
5	H	181	
6	K	435	
6	L	435	
6	M	435	




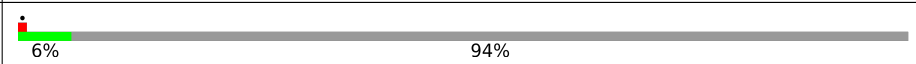
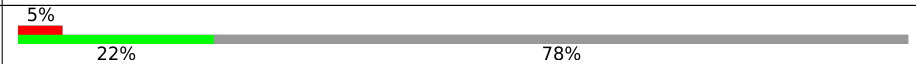
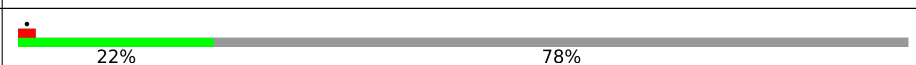

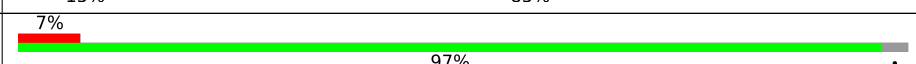
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Mol	Chain	Length	Quality of chain
7	J	177	 5% 99%
8	A	747	 5% 78% 22%
8	a	747	 5% 78% 22%
8	b	747	 5% 78% 22%
8	c	747	 5% 78% 22%
8	d	747	 5% 78% 22%
8	e	747	 5% 78% 22%
8	f	747	 5% 78% 22%
8	g	747	 5% 78% 22%
8	h	747	 5% 78% 22%
8	i	747	 5% 78% 22%
8	j	747	 5% 78% 22%
8	k	747	 5% 78% 22%
8	l	747	 5% 78% 22%
8	m	747	 5% 78% 22%
8	n	747	 5% 78% 22%
8	o	747	 5% 78% 22%
8	p	747	 6% 78% 22%
8	q	747	 7% 78% 22%
8	r	747	 5% 78% 22%
8	s	747	 5% 78% 22%
8	t	747	 5% 78% 22%
8	u	747	 5% 78% 22%
8	v	747	 5% 78% 22%
8	w	747	 5% 78% 22%

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Mol	Chain	Length	Quality of chain
8	x	747	 78% 22%
8	y	747	 78% 22%
8	z	747	 78% 22%
9	N	522	 6% 94%
9	O	522	 5% 22% 78%
9	P	522	 22% 78%
10	I	230	 11% 15% 85%
11	C	118	 7% 97%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 138685 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 gp28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	319	2563	1647	432	475	9	0	0

- Molecule 2 is a protein called gp35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	107	862	568	135	155	4	0	0

- Molecule 3 is a protein called gp85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	142	1102	698	190	211	3	0	0
3	F	141	1085	684	187	211	3	0	0

- Molecule 4 is a protein called gp86.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	297	2425	1547	423	447	8	0	0

- Molecule 5 is a protein called gp91.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	163	1333	857	226	245	5	0	0

- Molecule 6 is a protein called gp93.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	51	Total	C	N	O	0	0
			380	227	59	94		
6	L	71	Total	C	N	O	0	0
			528	320	80	128		
6	M	71	Total	C	N	O	0	0
			528	320	80	128		

- Molecule 7 is a protein called gp119.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	176	Total	C	N	O	S	0	0
			1416	903	236	272	5		

- Molecule 8 is a protein called gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	b	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	c	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	d	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	e	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	f	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	g	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	h	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	i	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	j	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	k	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	l	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	m	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	n	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	p	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	q	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	r	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	s	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	t	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	u	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	v	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	w	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	x	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	y	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	z	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	A	582	Total	C	N	O	S	0	0
			4550	2876	785	872	17		

- Molecule 9 is a protein called gp162.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	32	Total	C	N	O	0	0	
			246	151	36	59			
9	O	116	Total	C	N	O	S	0	0
			885	538	149	195	3		
9	P	116	Total	C	N	O	S	0	0
			885	538	149	195	3		

- Molecule 10 is a protein called gp184.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	34	Total	C	N	O	S	0	0
			272	171	42	58	1		

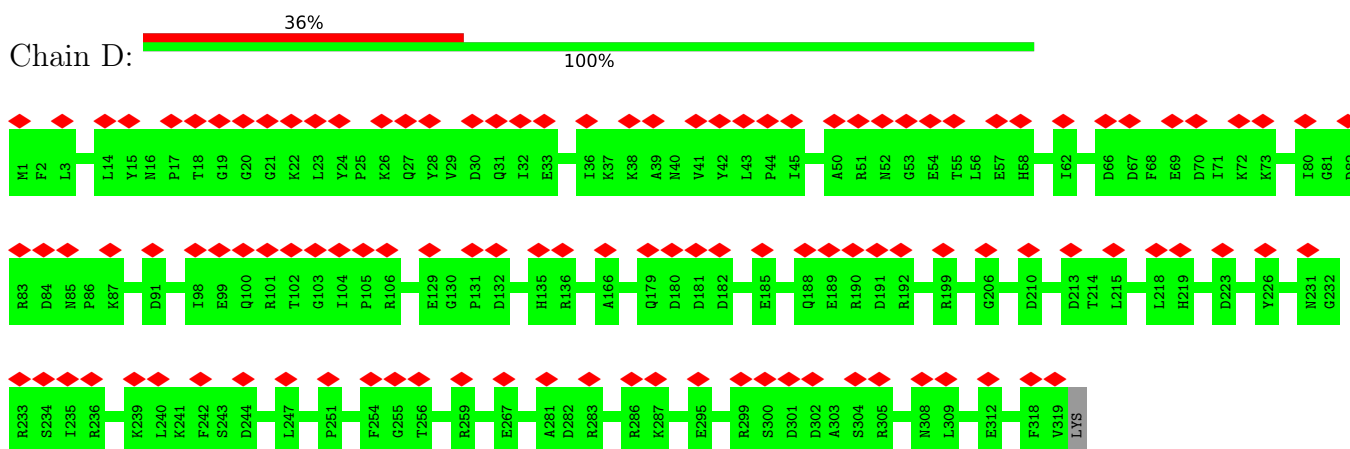
- Molecule 11 is a protein called gp244.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	114	909	571	149	184	5	0	0

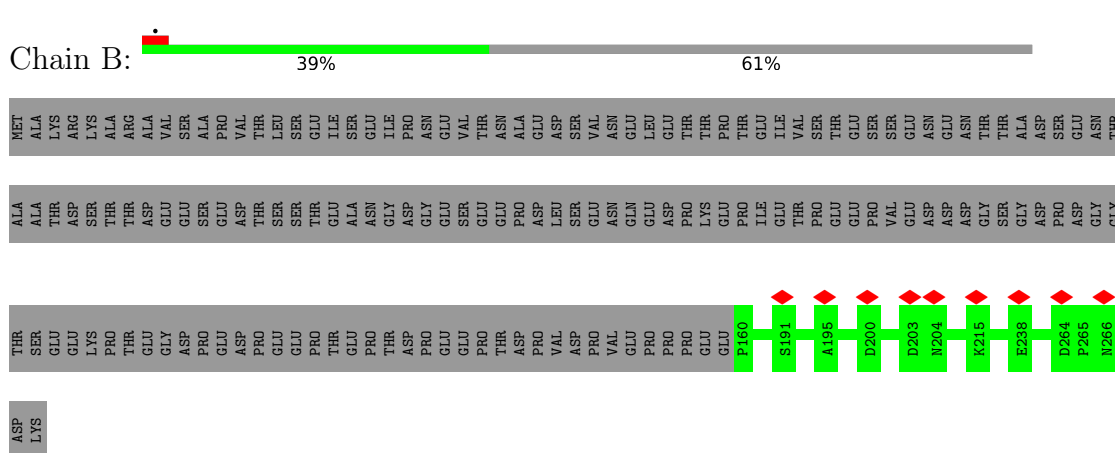
3 Residue-property plots

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.

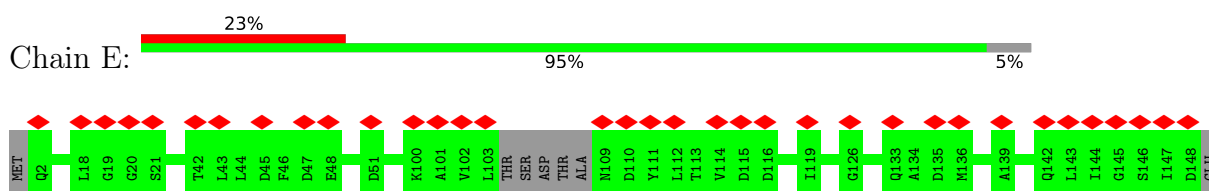
- Molecule 1: gp28



- Molecule 2: gp35

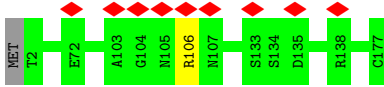


- Molecule 3: gp85

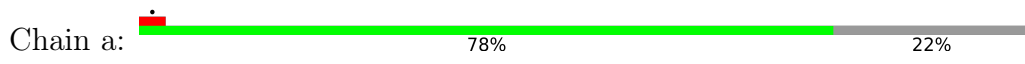


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• Molecule 7: gp119

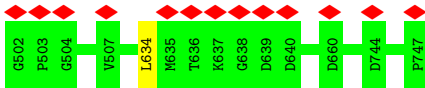
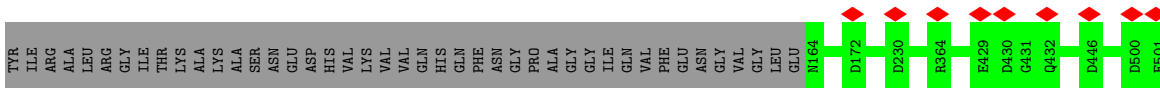


• Molecule 8: gp120

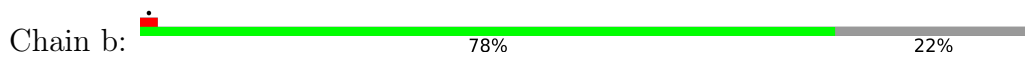


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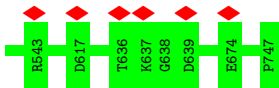
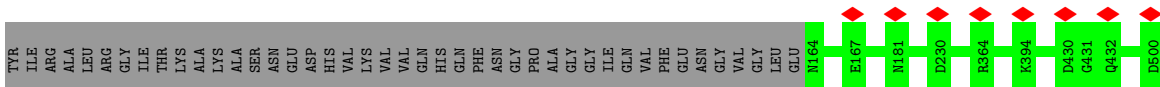


• Molecule 8: gp120

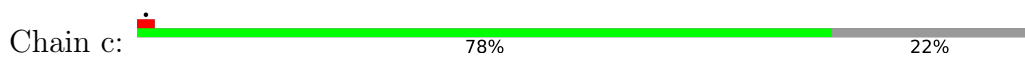


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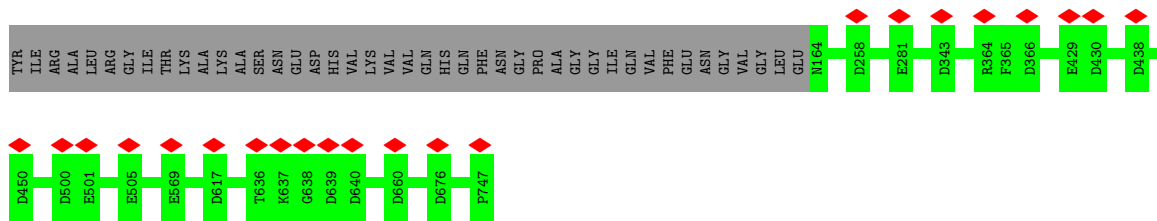


• Molecule 8: gp120

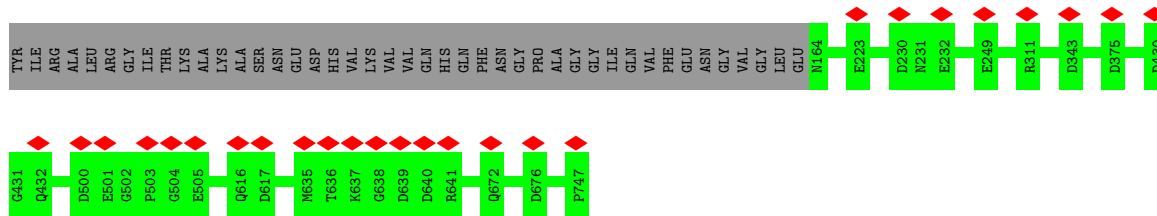
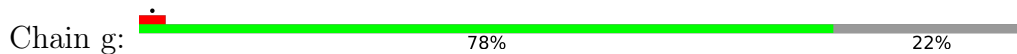


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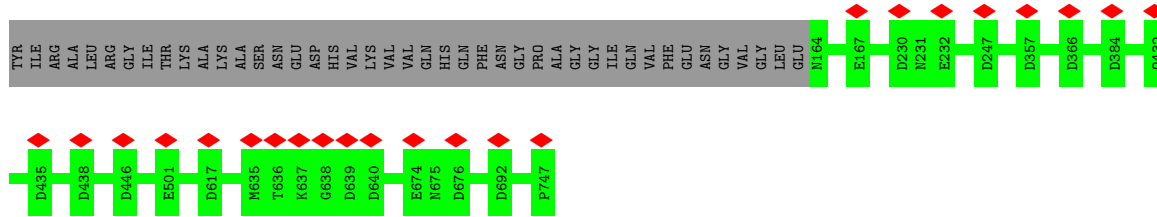
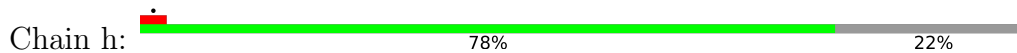
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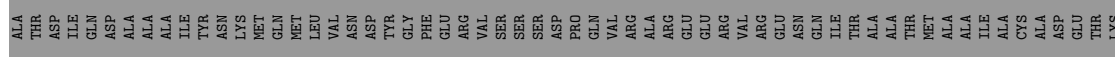
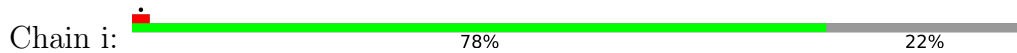
• Molecule 8: gp120

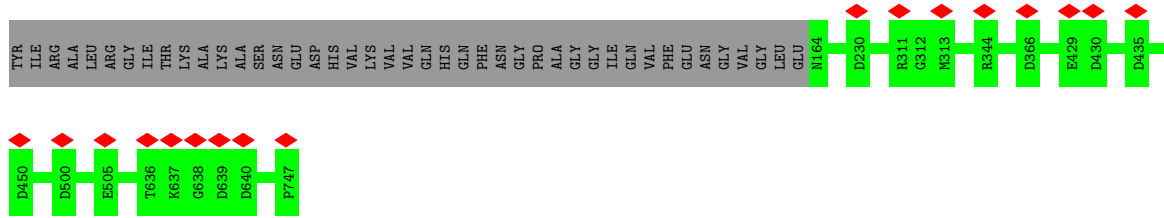


• Molecule 8: gp120

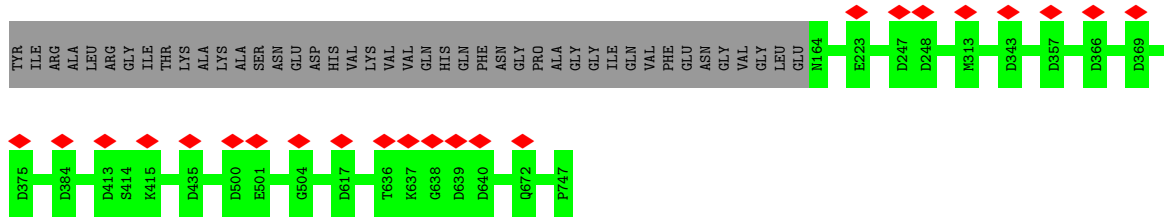
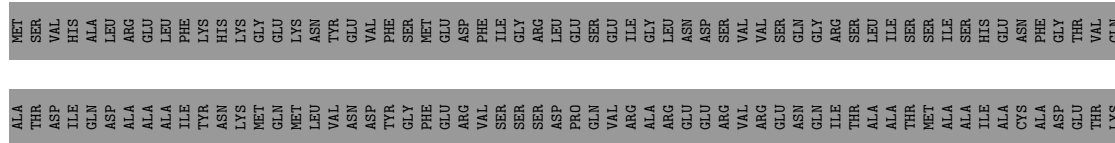
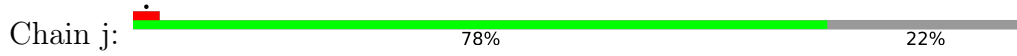


• Molecule 8: gp120

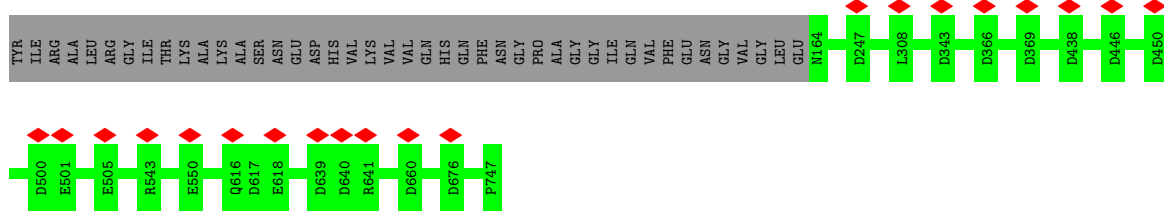
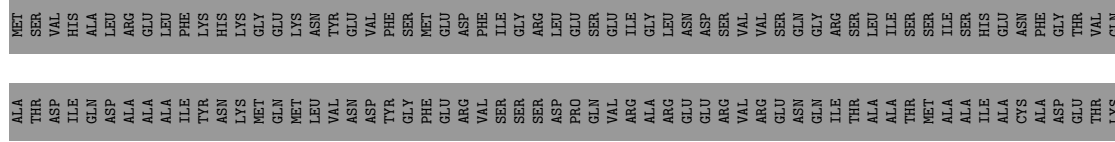
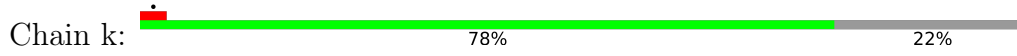




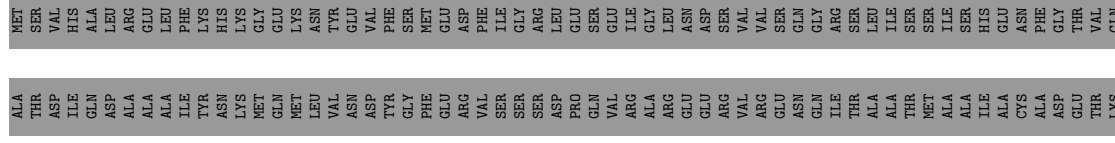
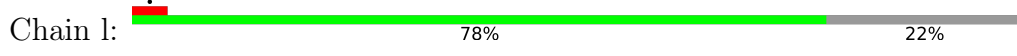
Molecule 8: gp120

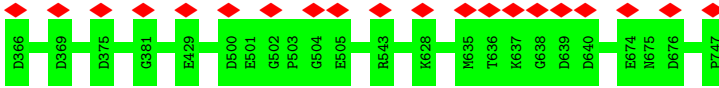
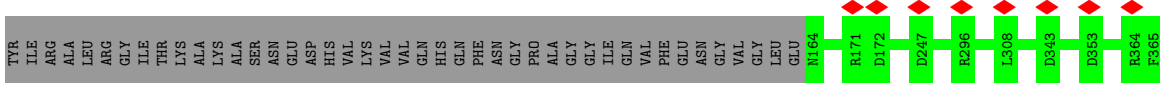


Molecule 8: gp120

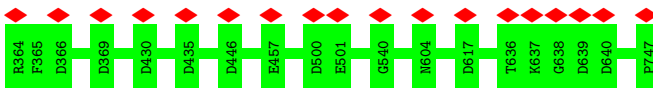
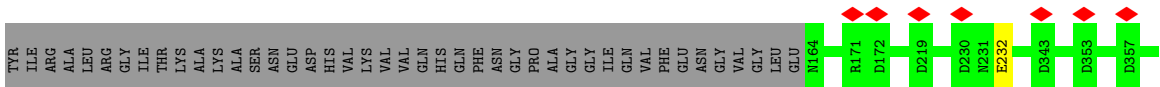
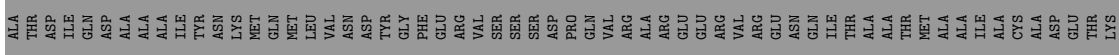
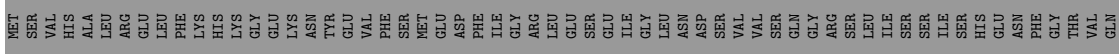
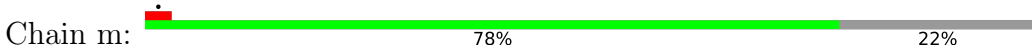


Molecule 8: gp120

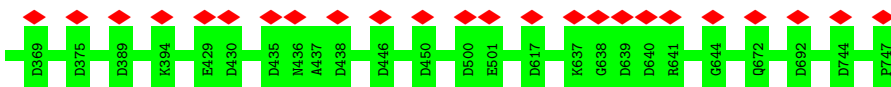
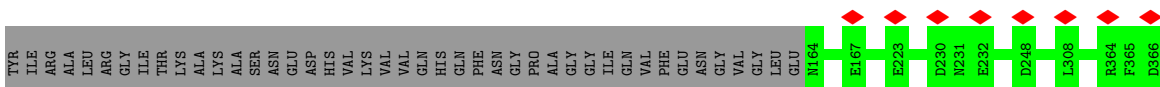
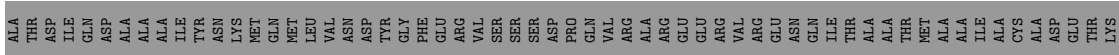
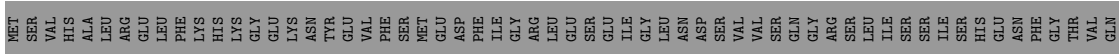
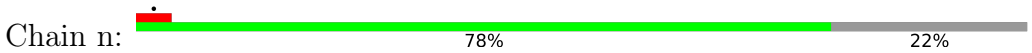




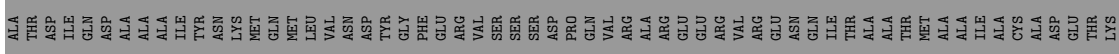
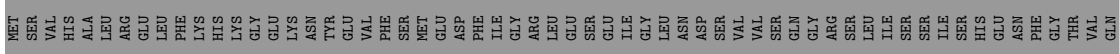
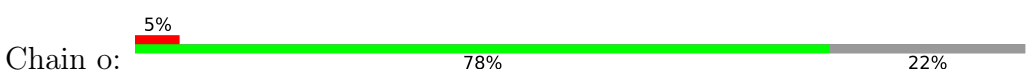
Molecule 8: gp120

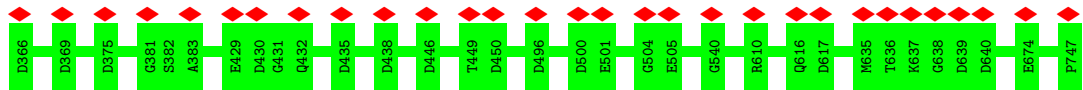
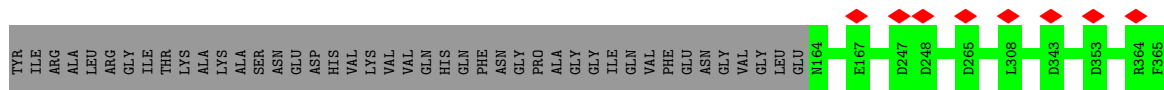


Molecule 8: gp120

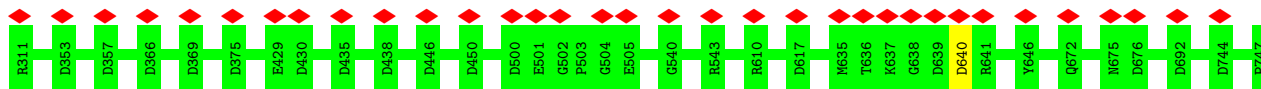
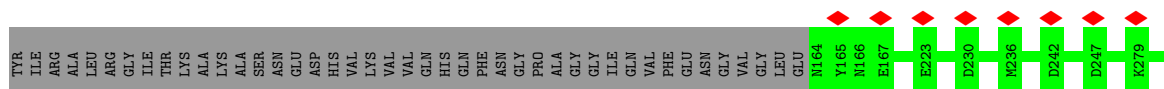
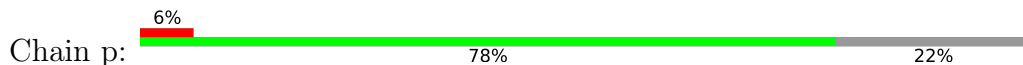


Molecule 8: gp120

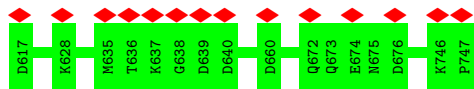
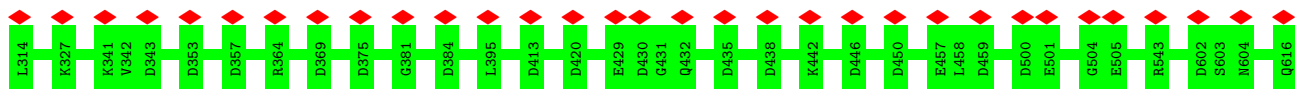
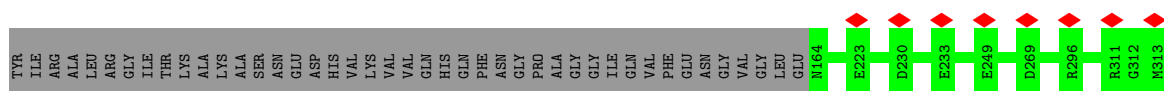
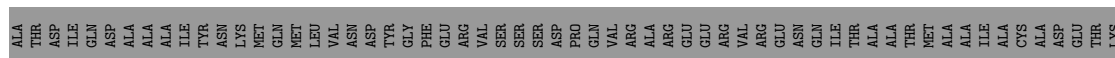
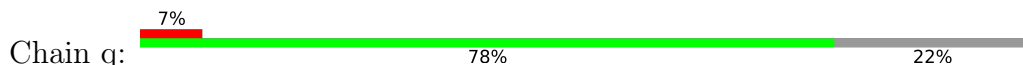




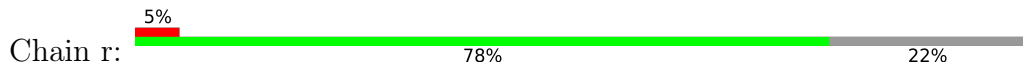
• Molecule 8: gp120

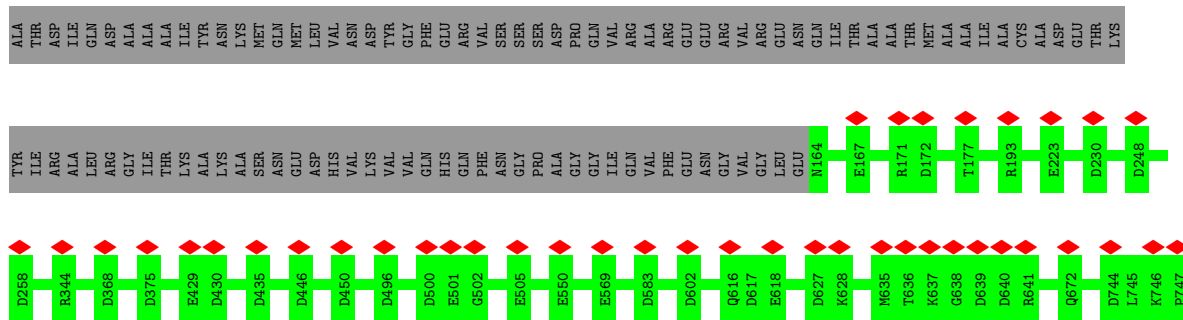


• Molecule 8: gp120

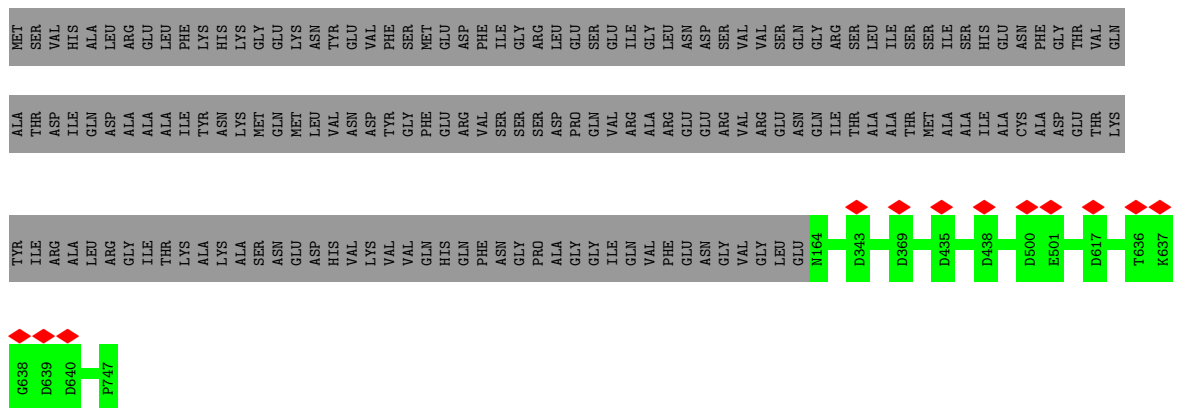
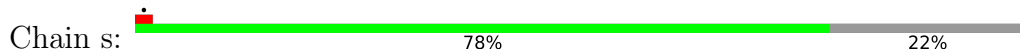


• Molecule 8: gp120

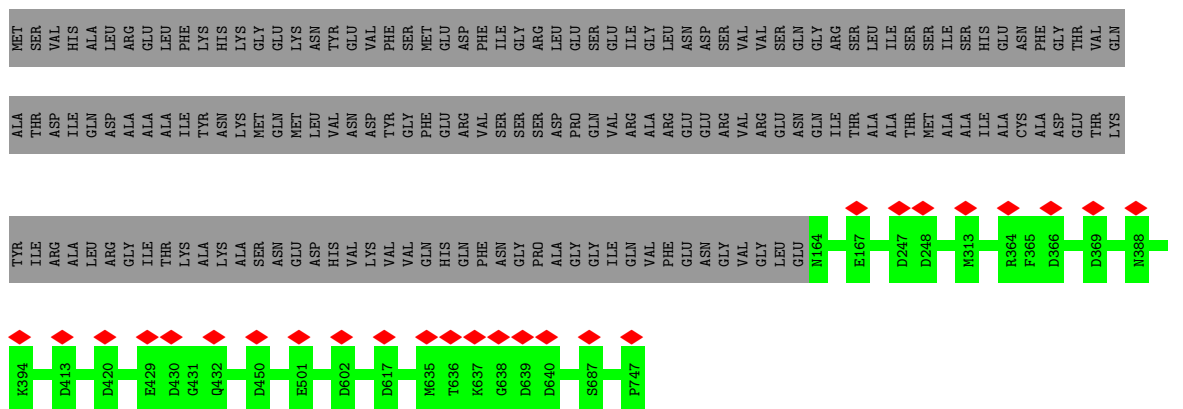
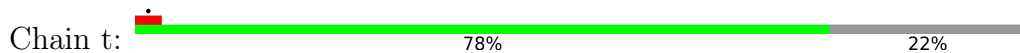




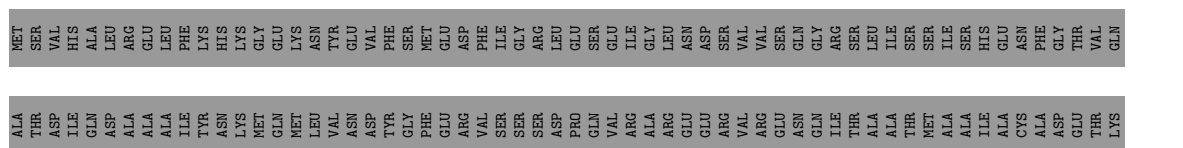
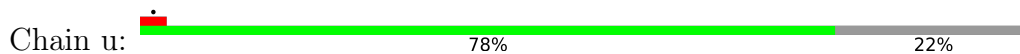
● Molecule 8: gp120

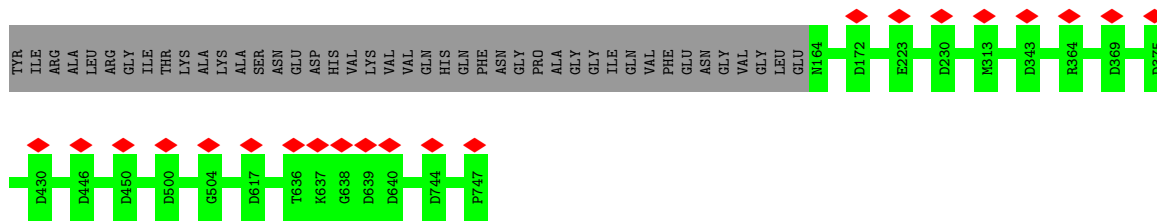


● Molecule 8: gp120

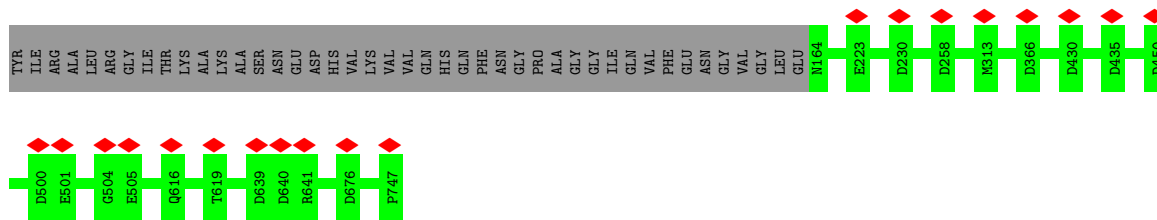
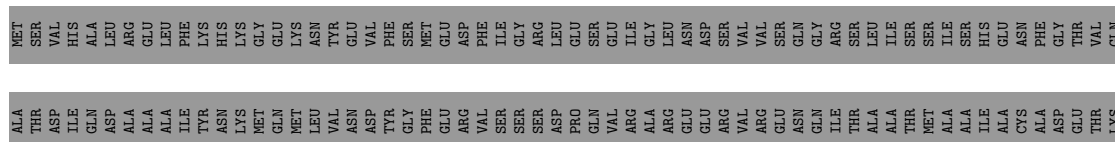
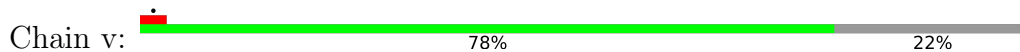


● Molecule 8: gp120

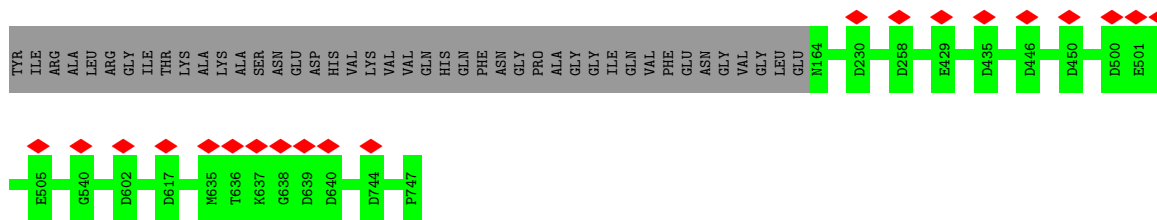
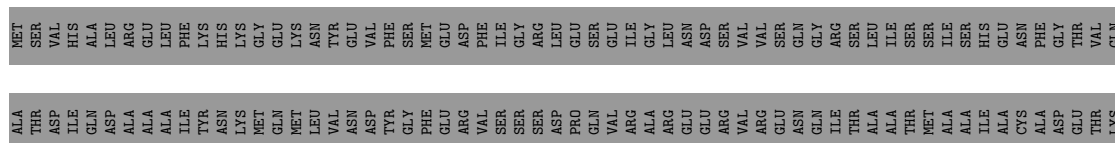
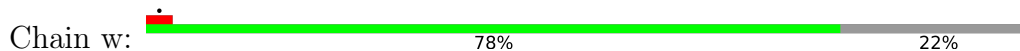




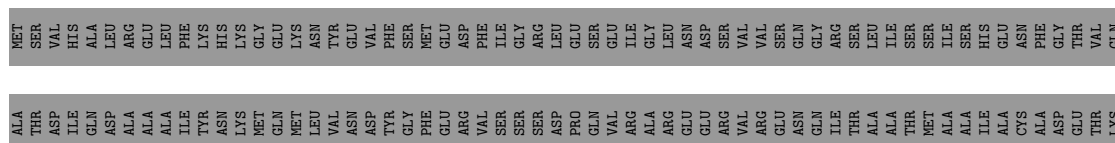
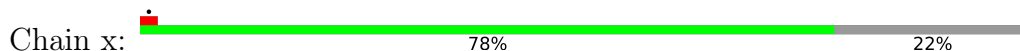
• Molecule 8: gp120

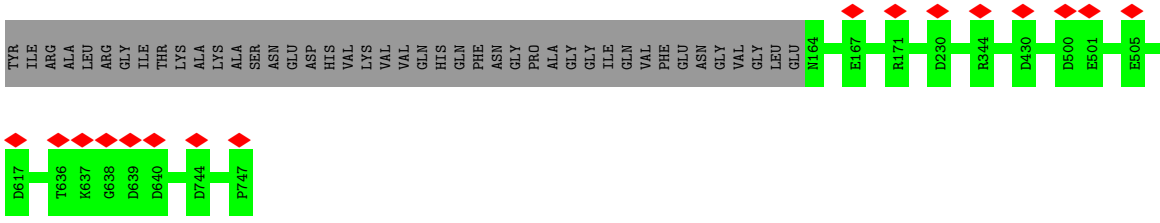


• Molecule 8: gp120

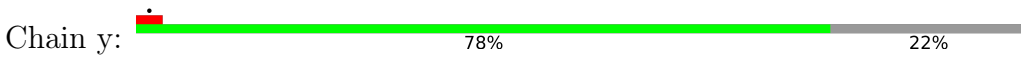


• Molecule 8: gp120

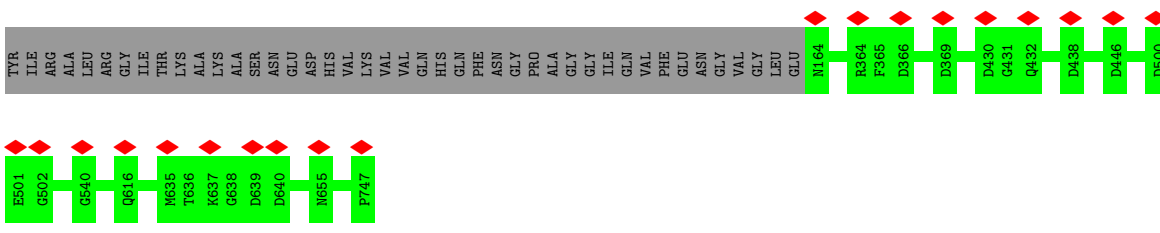




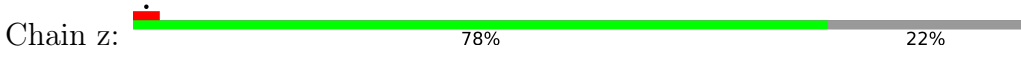
• Molecule 8: gp120



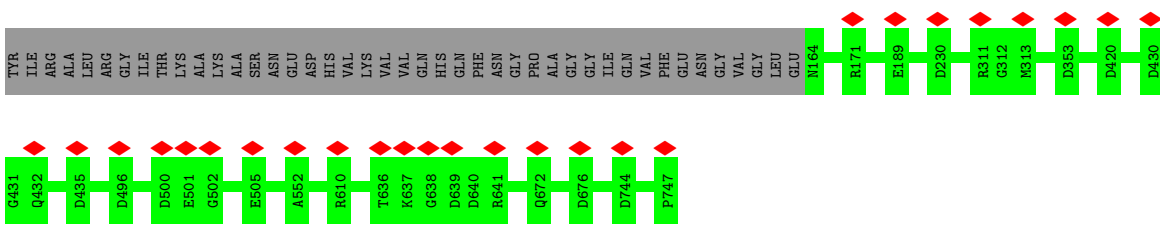
MET	SER	VAL	HIS	ALA	LEU	ARG	GLU	LEU	PHE	LYS	HIS	LYS	GLY	GLU	ASN	ASP	TYR	GLY	VAL	ASP	VAL	PHE	SER	GLY	GLN	MET	GLU	ASP	LEU	ASN	VAL	TYR	ASP	GLN	THR	PHE	TYR	GLY	VAL	GLY	GLU	GLN	GLY	ASP	LEU	LEU	GLY	GLY	GLY	VAL	VAL	VAL	VAL	VAL	GLN	ARG	GLY	ASP	ASN	GLY	THR	ILE	ALA	ALA	ALA	ALA	ILE	HIS	GLU	GLU	GLY	THR	THR	MET	SER	ILE	ALA	ALA	ALA	CYS	ASP	PHE	GLY	THR	THR	VAL	VAL	GLN	LYS
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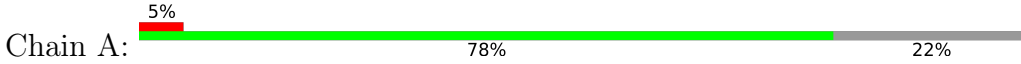
• Molecule 8: gp120



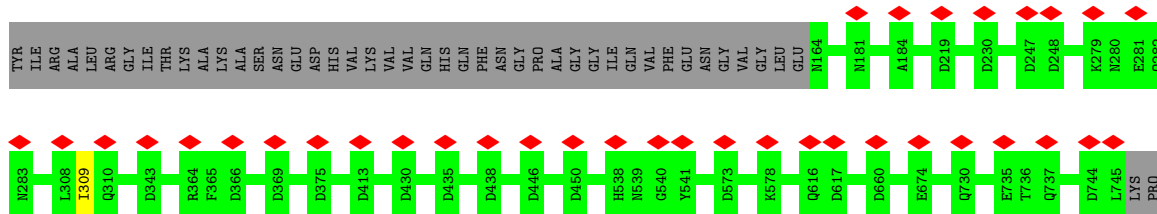
MET	SER	VAL	HIS	ALA	LEU	ARG	GLU	LEU	PHE	LYS	HIS	LYS	GLY	GLU	ASN	ASP	TYR	GLY	VAL	ASP	VAL	PHE	SER	GLY	GLN	MET	GLU	ASP	LEU	ASN	VAL	TYR	ASP	GLN	THR	PHE	TYR	GLY	VAL	GLY	GLU	GLN	GLY	ASP	LEU	LEU	GLY	GLY	GLY	VAL	VAL	VAL	VAL	VAL	GLN	ARG	GLY	ASP	ASN	GLY	THR	ILE	ALA	ALA	ALA	ALA	ILE	HIS	GLU	GLU	GLY	THR	THR	MET	SER	ILE	ALA	ALA	ALA	CYS	ASP	PHE	GLY	THR	THR	VAL	VAL	GLN	LYS
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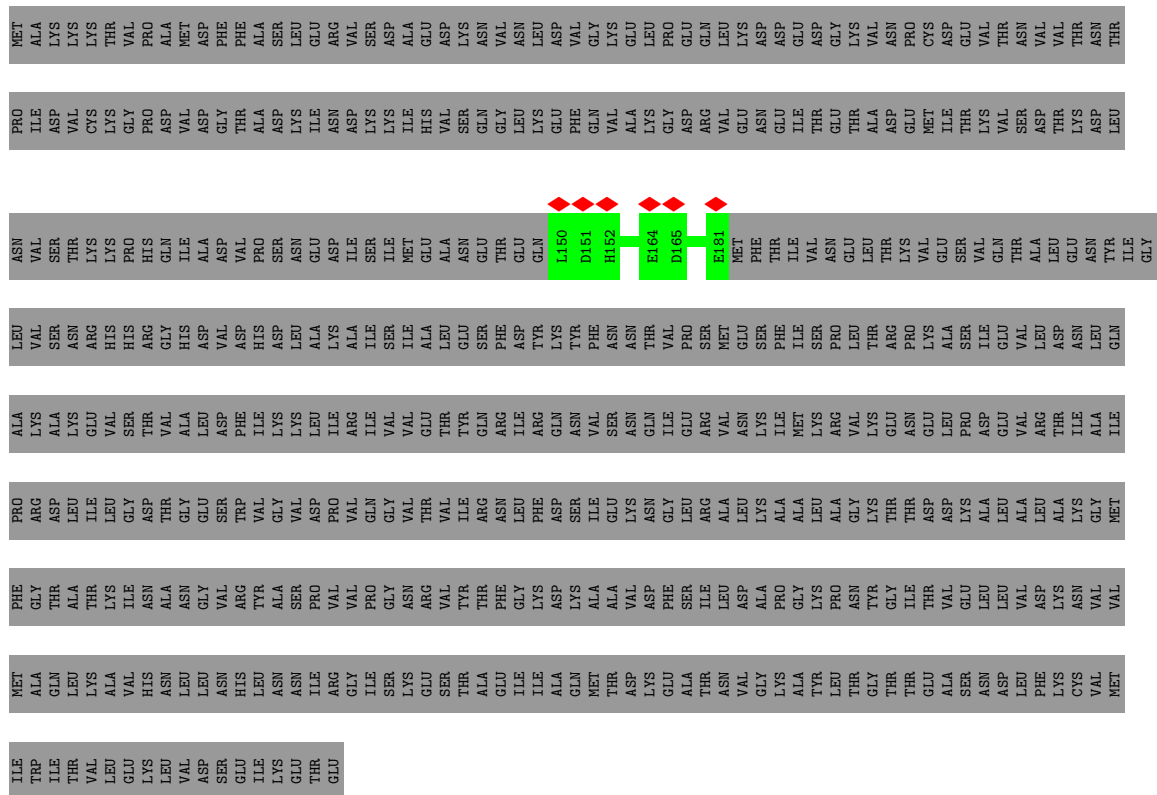
• Molecule 8: gp120



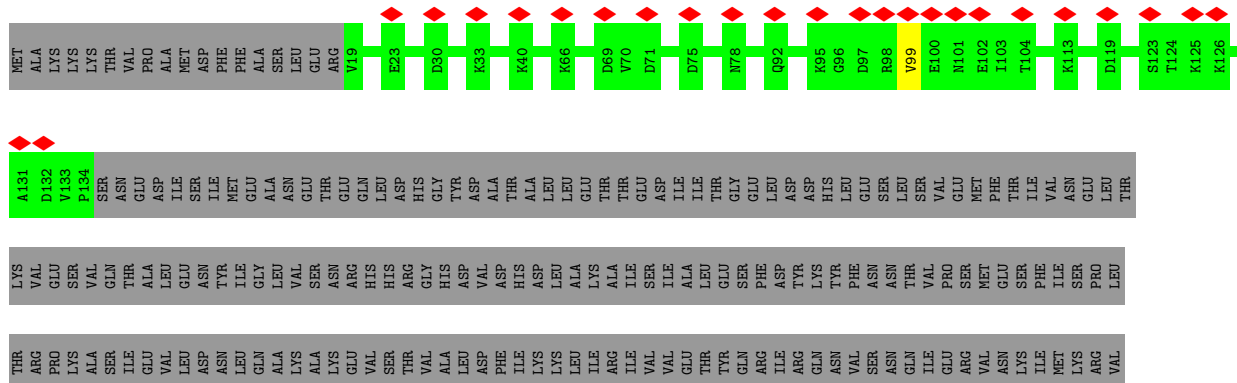
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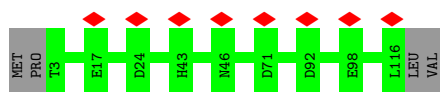


• Molecule 9: gp162



• Molecule 9: gp162





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	903900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0165	Depositor
Map size (Å)	1600.0, 1600.0, 1600.0	wwPDB
Map dimensions	1000, 1000, 1000	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6, 1.6, 1.6	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	D	0.60	0/2621	0.49	0/3561
2	B	0.55	0/887	0.51	0/1207
3	E	0.55	0/1112	0.50	0/1505
3	F	0.52	0/1095	0.50	0/1486
4	G	0.65	0/2467	0.50	0/3325
5	H	0.61	0/1367	0.49	0/1859
6	K	0.94	0/381	0.44	0/522
6	L	0.94	0/530	0.47	0/728
6	M	0.95	0/530	0.55	0/728
7	J	0.68	0/1445	0.51	0/1964
8	A	0.62	0/4631	0.52	0/6288
8	a	0.62	0/4648	0.52	0/6311
8	b	0.62	0/4648	0.50	0/6311
8	c	0.62	0/4648	0.51	0/6311
8	d	0.61	0/4648	0.49	0/6311
8	e	0.62	0/4648	0.49	0/6311
8	f	0.62	0/4648	0.51	0/6311
8	g	0.62	0/4648	0.50	0/6311
8	h	0.62	0/4648	0.51	0/6311
8	i	0.61	0/4648	0.50	0/6311
8	j	0.62	0/4648	0.50	0/6311
8	k	0.62	0/4648	0.50	0/6311
8	l	0.61	0/4648	0.49	0/6311
8	m	0.60	0/4648	0.51	0/6311
8	n	0.62	0/4648	0.50	0/6311
8	o	0.62	0/4648	0.51	0/6311
8	p	0.62	0/4648	0.50	0/6311
8	q	0.62	0/4648	0.49	0/6311
8	r	0.62	0/4648	0.50	0/6311
8	s	0.63	0/4648	0.49	0/6311
8	t	0.62	0/4648	0.52	0/6311
8	u	0.62	0/4648	0.49	0/6311
8	v	0.63	0/4648	0.50	0/6311
8	w	0.62	0/4648	0.50	0/6311

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	x	0.63	0/4648	0.49	0/6311
8	y	0.62	0/4648	0.50	0/6311
8	z	0.62	0/4648	0.50	0/6311
9	N	0.93	0/248	0.51	0/338
9	O	0.74	0/893	0.54	0/1210
9	P	0.79	0/893	0.60	0/1210
10	I	0.33	0/281	0.48	0/387
11	C	0.64	0/924	0.49	0/1249
All	All	0.63	0/141153	0.50	0/191653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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	D	317/320 (99%)	313 (99%)	4 (1%)	0	100	100
2	B	105/271 (39%)	101 (96%)	4 (4%)	0	100	100
3	E	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
3	F	139/149 (93%)	136 (98%)	3 (2%)	0	100	100
4	G	293/428 (68%)	285 (97%)	6 (2%)	2 (1%)	22	61
5	H	161/181 (89%)	154 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	49/435 (11%)	48 (98%)	1 (2%)	0	100	100
6	L	69/435 (16%)	63 (91%)	6 (9%)	0	100	100
6	M	69/435 (16%)	66 (96%)	3 (4%)	0	100	100
7	J	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	25	64
8	A	580/747 (78%)	562 (97%)	17 (3%)	1 (0%)	47	81
8	a	582/747 (78%)	564 (97%)	17 (3%)	1 (0%)	47	81
8	b	582/747 (78%)	569 (98%)	13 (2%)	0	100	100
8	c	582/747 (78%)	555 (95%)	24 (4%)	3 (0%)	29	68
8	d	582/747 (78%)	564 (97%)	18 (3%)	0	100	100
8	e	582/747 (78%)	561 (96%)	20 (3%)	1 (0%)	47	81
8	f	582/747 (78%)	565 (97%)	17 (3%)	0	100	100
8	g	582/747 (78%)	568 (98%)	14 (2%)	0	100	100
8	h	582/747 (78%)	567 (97%)	15 (3%)	0	100	100
8	i	582/747 (78%)	563 (97%)	19 (3%)	0	100	100
8	j	582/747 (78%)	561 (96%)	21 (4%)	0	100	100
8	k	582/747 (78%)	566 (97%)	16 (3%)	0	100	100
8	l	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	m	582/747 (78%)	563 (97%)	18 (3%)	1 (0%)	47	81
8	n	582/747 (78%)	573 (98%)	9 (2%)	0	100	100
8	o	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	p	582/747 (78%)	568 (98%)	13 (2%)	1 (0%)	47	81
8	q	582/747 (78%)	572 (98%)	10 (2%)	0	100	100
8	r	582/747 (78%)	566 (97%)	16 (3%)	0	100	100
8	s	582/747 (78%)	572 (98%)	10 (2%)	0	100	100
8	t	582/747 (78%)	554 (95%)	28 (5%)	0	100	100
8	u	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	v	582/747 (78%)	574 (99%)	8 (1%)	0	100	100
8	w	582/747 (78%)	572 (98%)	10 (2%)	0	100	100
8	x	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	y	582/747 (78%)	571 (98%)	11 (2%)	0	100	100
8	z	582/747 (78%)	574 (99%)	8 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	30/522 (6%)	30 (100%)	0	0	100	100
9	O	114/522 (22%)	104 (91%)	9 (8%)	1 (1%)	17	56
9	P	114/522 (22%)	102 (90%)	11 (10%)	1 (1%)	17	56
10	I	32/230 (14%)	29 (91%)	3 (9%)	0	100	100
11	C	112/118 (95%)	112 (100%)	0	0	100	100
All	All	17628/25063 (70%)	17148 (97%)	467 (3%)	13 (0%)	54	84

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	P	103	ILE
8	c	226	GLY
8	c	227	VAL
8	m	232	GLU
4	G	333	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	283/284 (100%)	283 (100%)	0	100	100
2	B	95/242 (39%)	95 (100%)	0	100	100
3	E	123/129 (95%)	123 (100%)	0	100	100
3	F	122/129 (95%)	122 (100%)	0	100	100
4	G	260/374 (70%)	260 (100%)	0	100	100
5	H	143/157 (91%)	143 (100%)	0	100	100
6	K	45/365 (12%)	45 (100%)	0	100	100
6	L	62/365 (17%)	62 (100%)	0	100	100
6	M	62/365 (17%)	62 (100%)	0	100	100
7	J	159/160 (99%)	159 (100%)	0	100	100
8	A	501/638 (78%)	501 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	a	503/638 (79%)	503 (100%)	0	100	100
8	b	503/638 (79%)	503 (100%)	0	100	100
8	c	503/638 (79%)	503 (100%)	0	100	100
8	d	503/638 (79%)	503 (100%)	0	100	100
8	e	503/638 (79%)	503 (100%)	0	100	100
8	f	503/638 (79%)	503 (100%)	0	100	100
8	g	503/638 (79%)	503 (100%)	0	100	100
8	h	503/638 (79%)	503 (100%)	0	100	100
8	i	503/638 (79%)	503 (100%)	0	100	100
8	j	503/638 (79%)	503 (100%)	0	100	100
8	k	503/638 (79%)	503 (100%)	0	100	100
8	l	503/638 (79%)	503 (100%)	0	100	100
8	m	503/638 (79%)	503 (100%)	0	100	100
8	n	503/638 (79%)	503 (100%)	0	100	100
8	o	503/638 (79%)	503 (100%)	0	100	100
8	p	503/638 (79%)	503 (100%)	0	100	100
8	q	503/638 (79%)	503 (100%)	0	100	100
8	r	503/638 (79%)	503 (100%)	0	100	100
8	s	503/638 (79%)	503 (100%)	0	100	100
8	t	503/638 (79%)	503 (100%)	0	100	100
8	u	503/638 (79%)	503 (100%)	0	100	100
8	v	503/638 (79%)	503 (100%)	0	100	100
8	w	503/638 (79%)	503 (100%)	0	100	100
8	x	503/638 (79%)	503 (100%)	0	100	100
8	y	503/638 (79%)	503 (100%)	0	100	100
8	z	503/638 (79%)	503 (100%)	0	100	100
9	N	28/456 (6%)	28 (100%)	0	100	100
9	O	105/456 (23%)	105 (100%)	0	100	100
9	P	105/456 (23%)	105 (100%)	0	100	100
10	I	30/193 (16%)	30 (100%)	0	100	100
11	C	105/109 (96%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15306/21466 (71%)	15306 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
8	k	222	HIS
8	n	737	GLN
8	A	464	ASN
8	n	632	ASN
8	q	164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

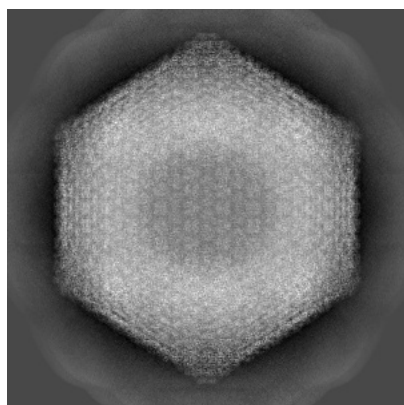
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39002. These allow visual inspection of the internal detail of the map and identification of artifacts.

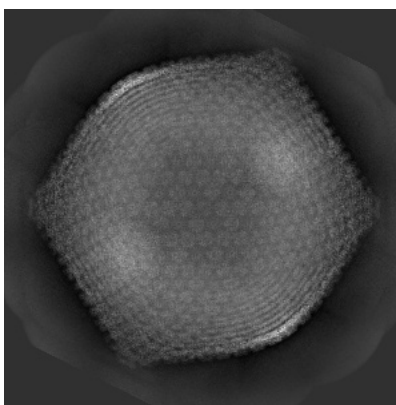
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

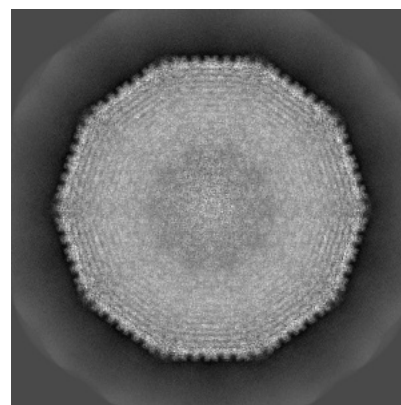
6.1.1 Primary map



X



Y

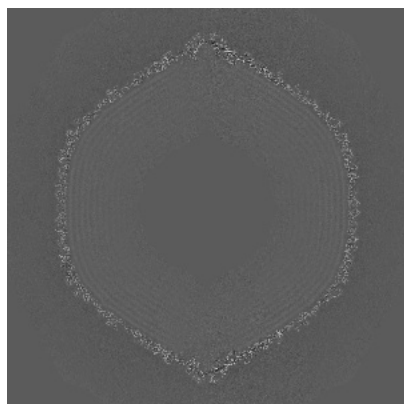


Z

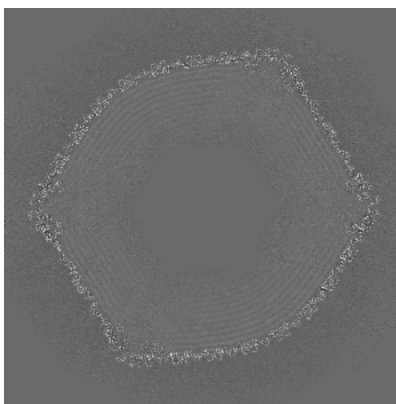
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

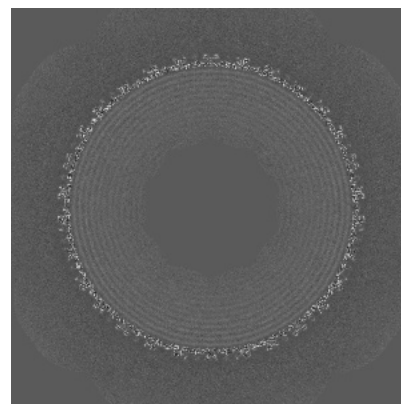
6.2.1 Primary map



X Index: 500



Y Index: 500

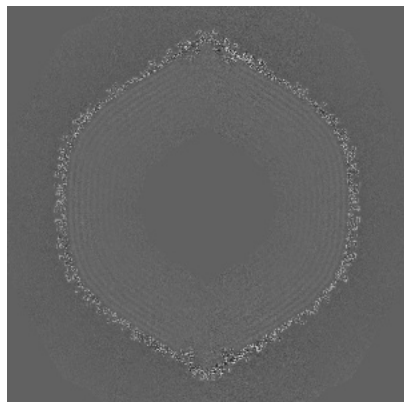


Z Index: 500

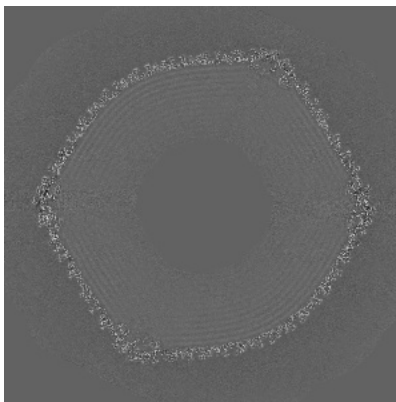
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

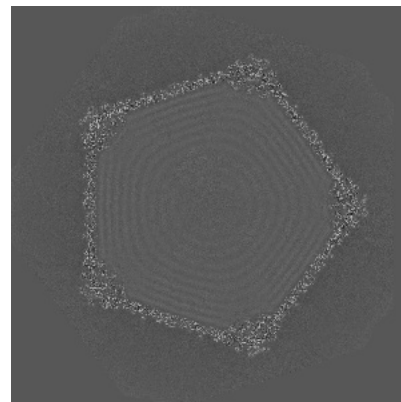
6.3.1 Primary map



X Index: 507



Y Index: 531

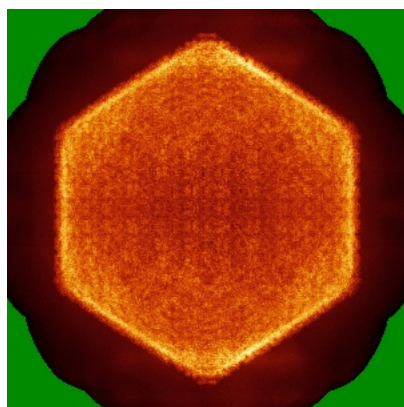


Z Index: 703

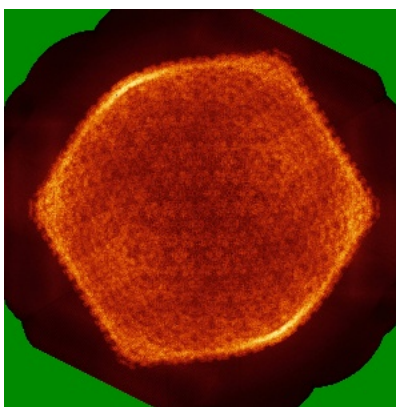
The images above show the largest variance slices of the map in three orthogonal directions.

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

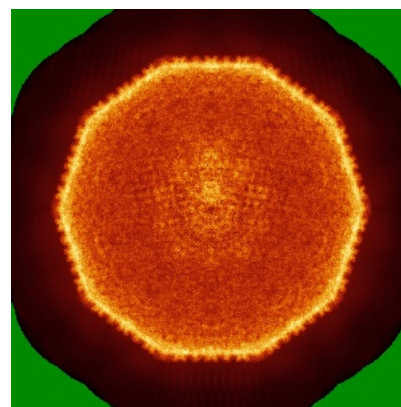
6.4.1 Primary map



X



Y

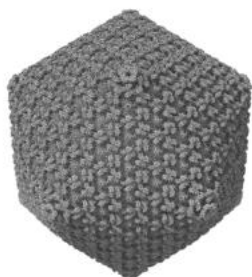


Z

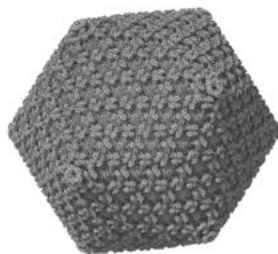
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

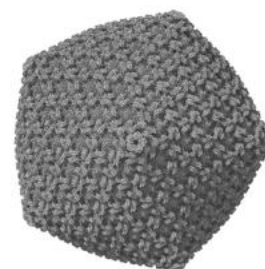
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

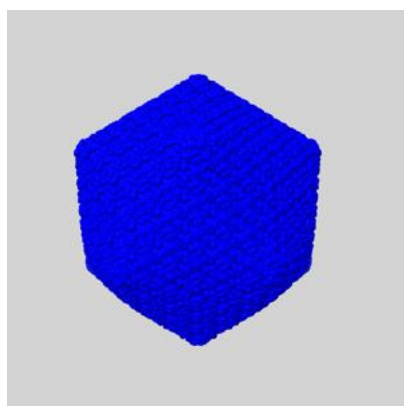
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

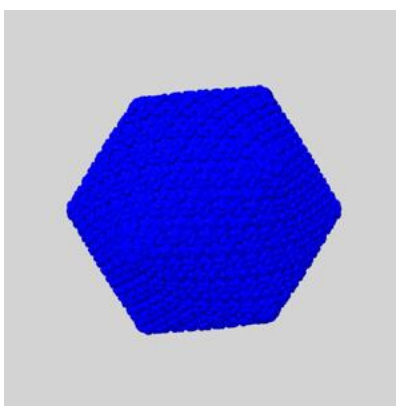
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

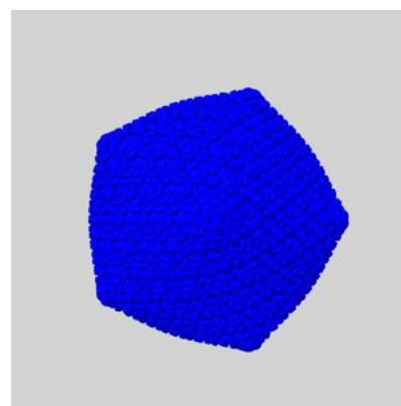
6.6.1 emd_39002_msk_1.map [i](#)



X



Y

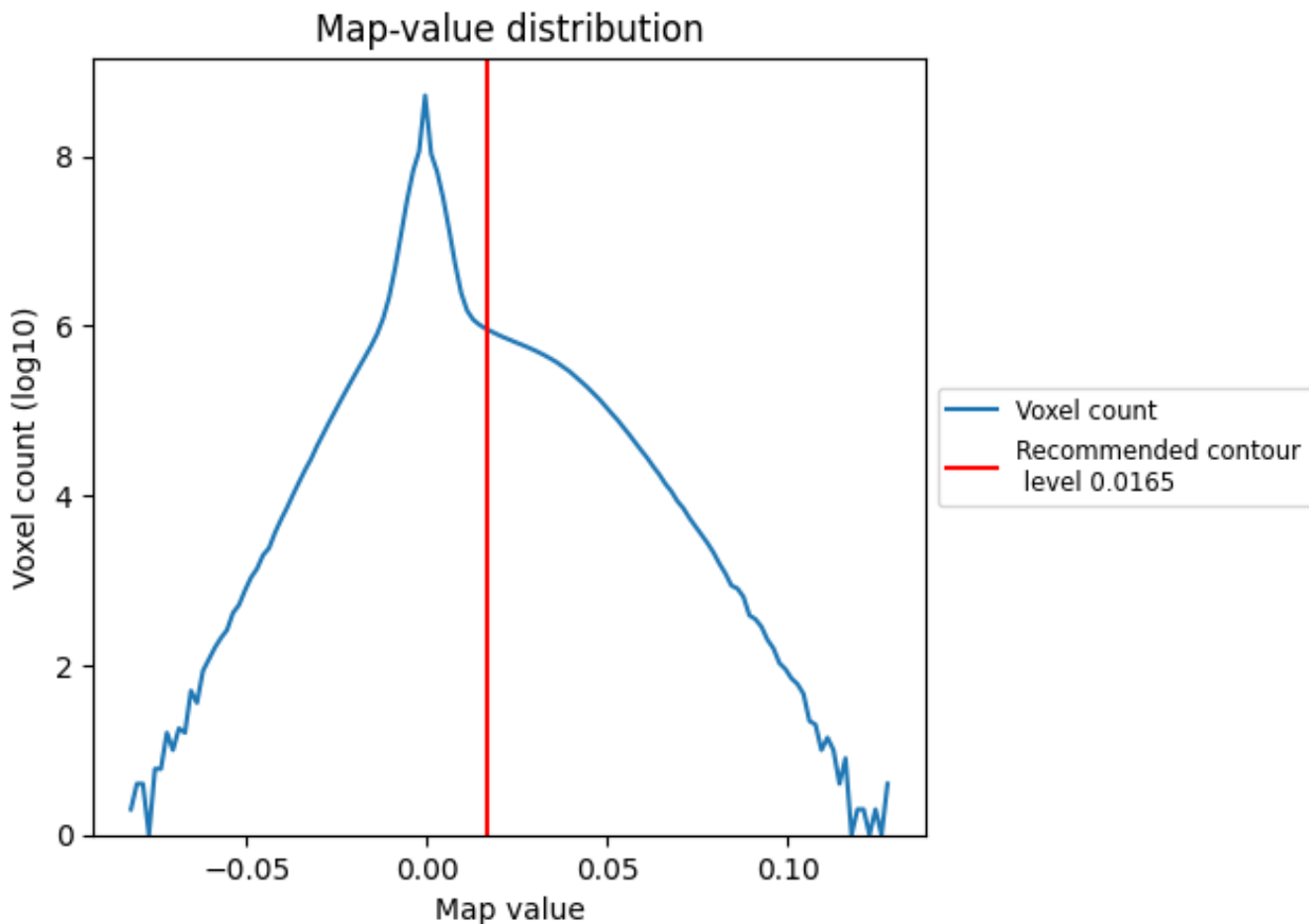


Z

7 Map analysis [i](#)

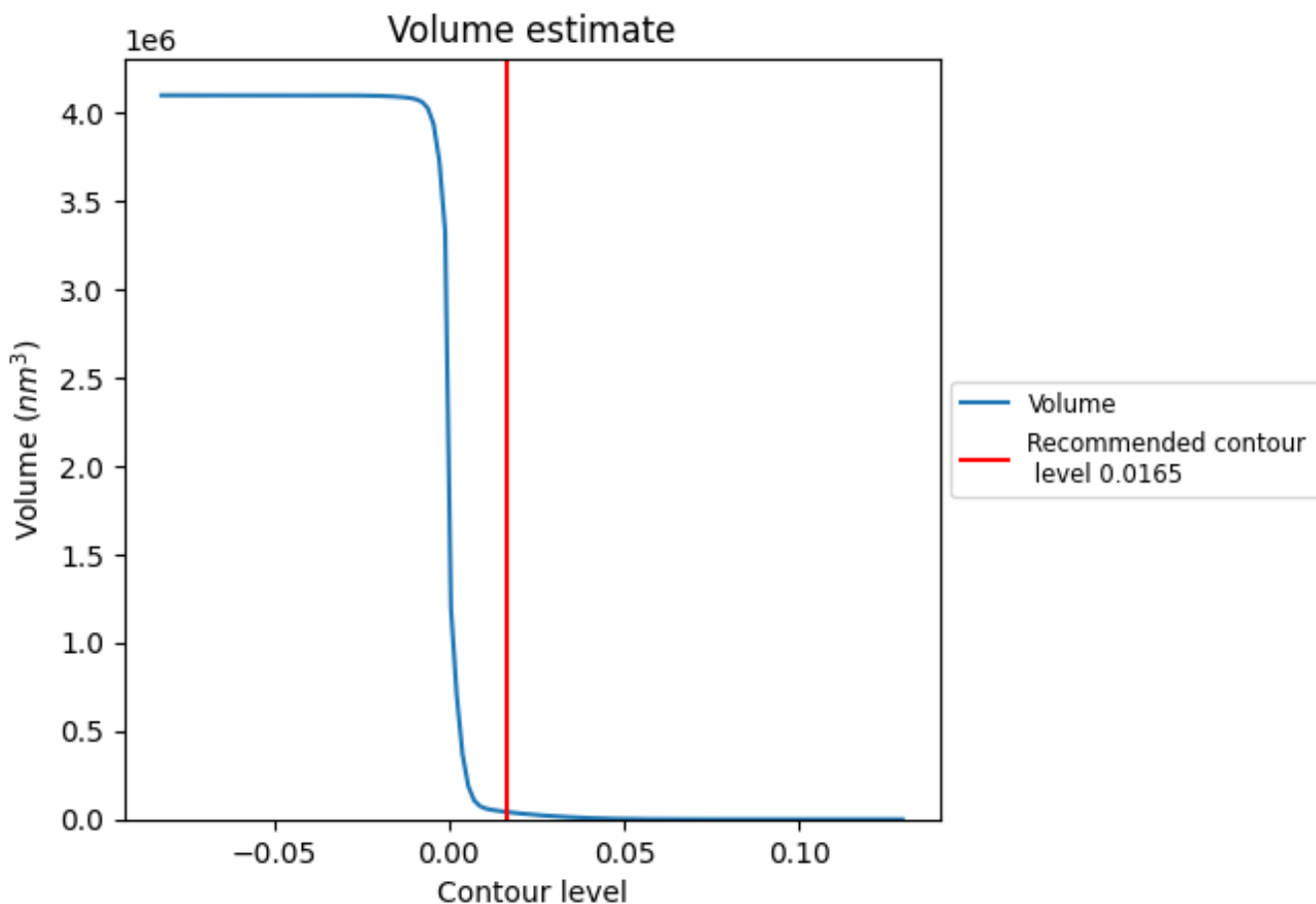
This section contains the results of statistical analysis of the map.

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.

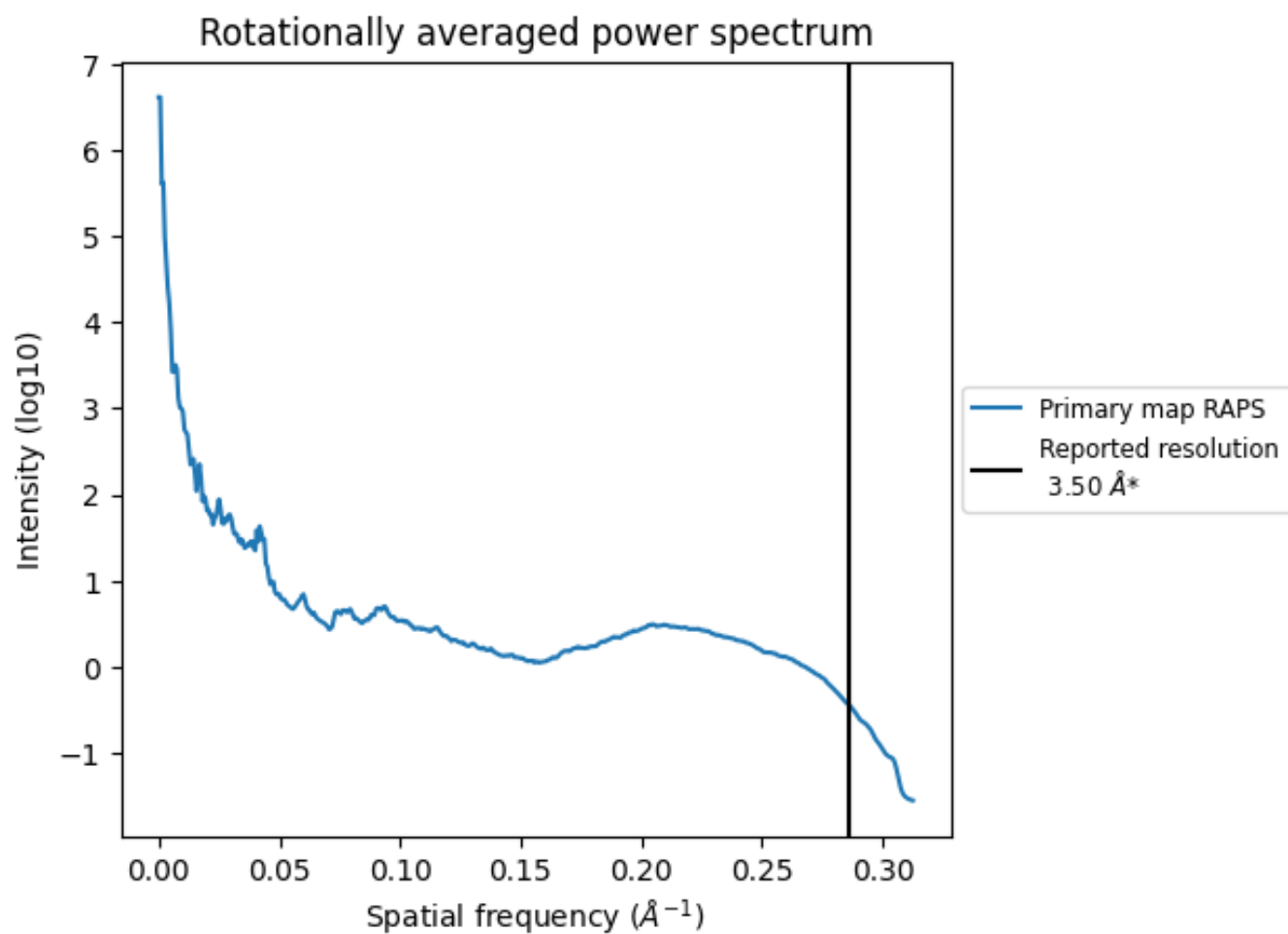
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 41513 nm³; this corresponds to an approximate mass of 37499 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation

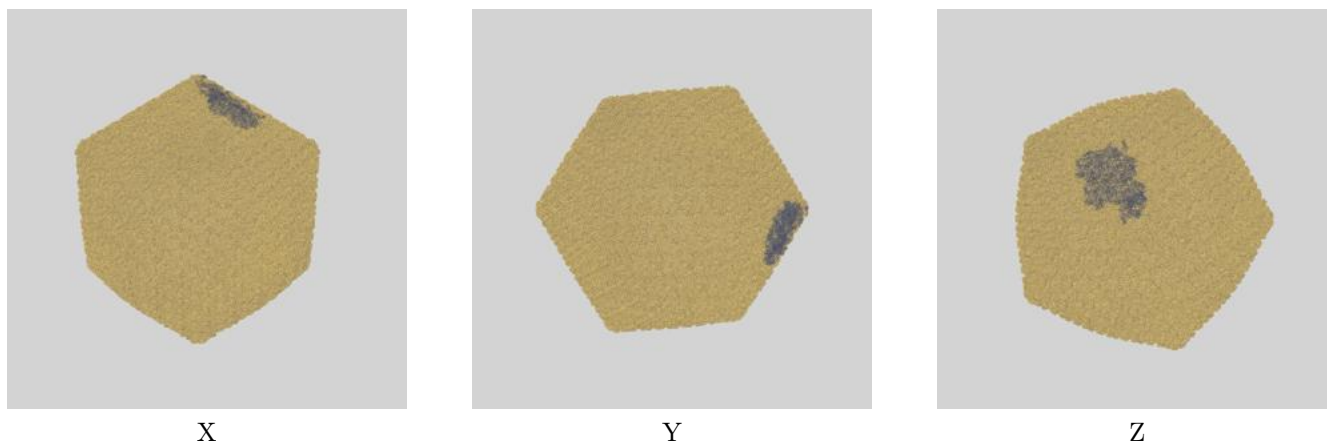
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

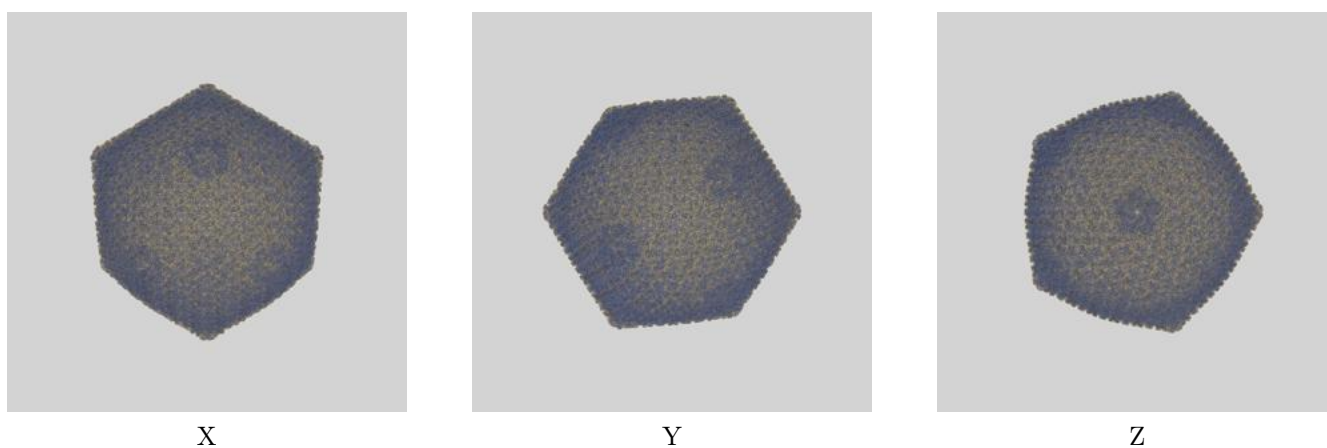
This section contains information regarding the fit between EMDB map EMD-39002 and PDB model 8Y6V. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

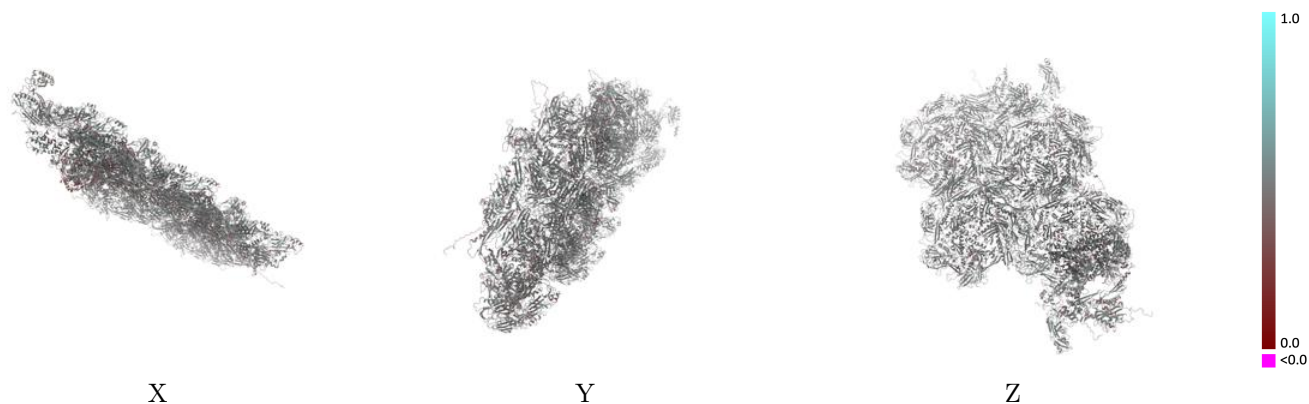


9.1.2 Map-model assembly overlay [i](#)



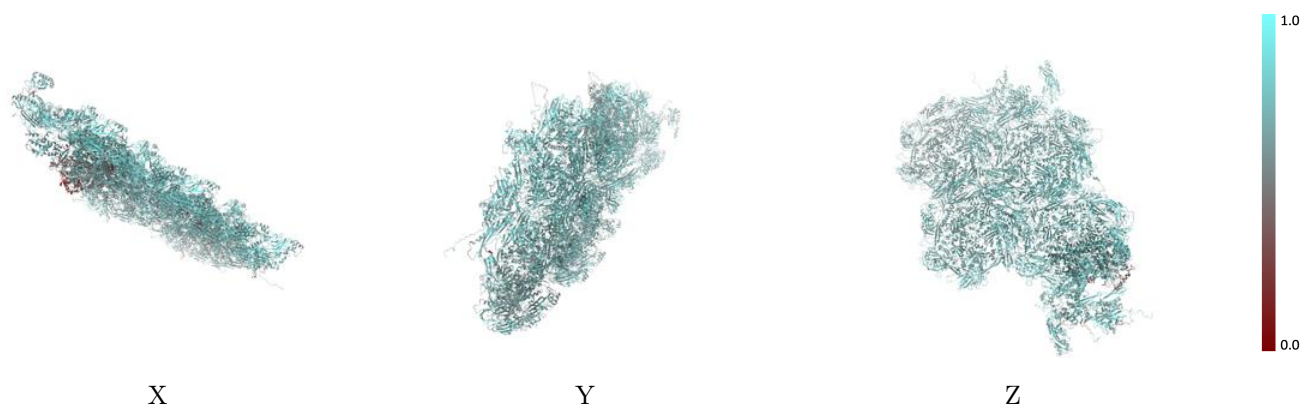
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



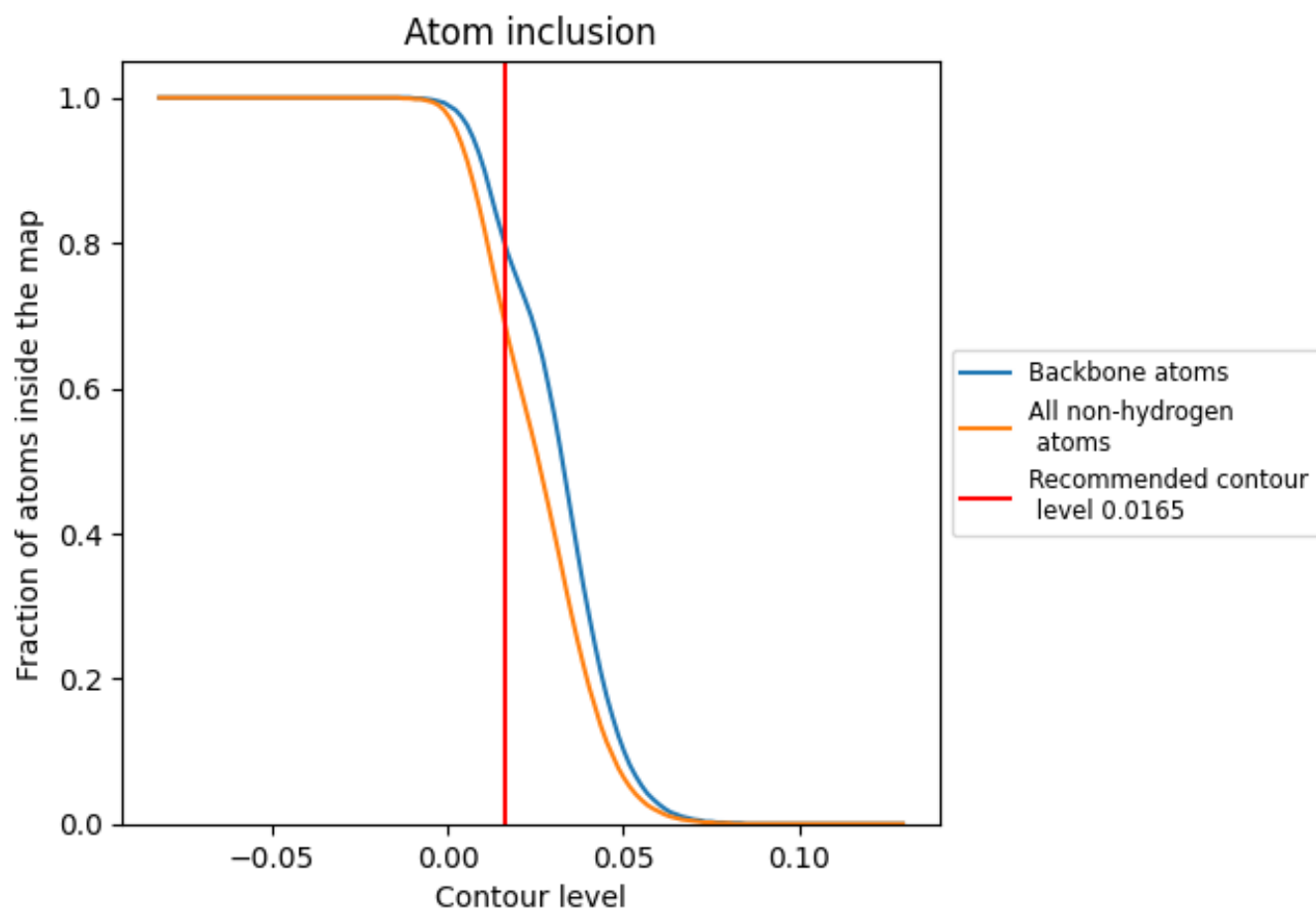
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0165).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.4610
A	 0.6840	 0.4650
B	 0.6710	 0.4640
C	 0.6490	 0.4460
D	 0.4730	 0.4310
E	 0.5480	 0.4110
F	 0.4090	 0.3750
G	 0.6050	 0.4360
H	 0.6290	 0.4550
I	 0.2650	 0.4210
J	 0.6670	 0.4620
K	 0.5550	 0.4110
L	 0.6210	 0.4290
M	 0.6000	 0.4280
N	 0.5880	 0.4230
O	 0.5270	 0.3970
P	 0.5610	 0.4120
a	 0.7260	 0.4690
b	 0.7310	 0.4710
c	 0.7390	 0.4660
d	 0.7380	 0.4670
e	 0.7290	 0.4700
f	 0.7340	 0.4740
g	 0.6980	 0.4640
h	 0.7080	 0.4630
i	 0.7060	 0.4730
j	 0.7000	 0.4710
k	 0.6900	 0.4620
l	 0.6870	 0.4590
m	 0.6820	 0.4670
n	 0.6920	 0.4670
o	 0.6500	 0.4570
p	 0.6190	 0.4530
q	 0.6110	 0.4480
r	 0.6360	 0.4540



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Chain	Atom inclusion	Q-score
s	 0.7390	 0.4680
t	 0.7140	 0.4630
u	 0.7010	 0.4760
v	 0.7010	 0.4700
w	 0.7040	 0.4640
x	 0.7270	 0.4700
y	 0.7110	 0.4670
z	 0.6820	 0.4620