



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 06:13 AM EST

PDB ID : 6OJ5
EMDB ID : EMD-20088
Title : In situ structure of rotavirus VP1 RNA-dependent RNA polymerase (TLP_RNA)
Authors : Jenni, S.; Salgado, E.N.; Herrmann, T.; Li, Z.; Grant, T.; Grigorieff, N.; Trapani, S.; Estrozi, L.F.; Harrison, S.C.
Deposited on : 2019-04-10
Resolution : 5.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

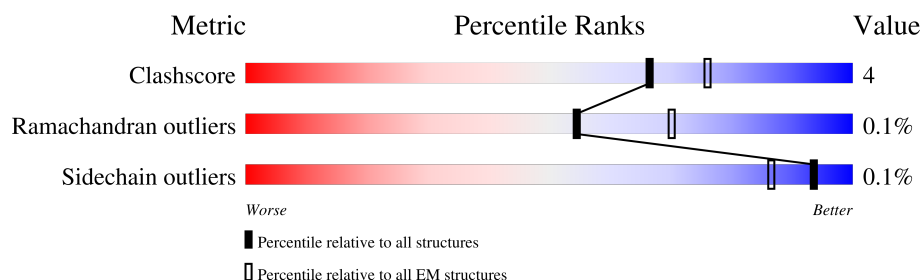
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	887	<div> <div>52%</div> <div>76% 12% 12%</div> </div>
1	B	887	<div> <div>46%</div> <div>75% 13% 12%</div> </div>
1	C	887	<div> <div>41%</div> <div>75% 13% 12%</div> </div>
1	D	887	<div> <div>50%</div> <div>81% 12% 7%</div> </div>
1	E	887	<div> <div>50%</div> <div>78% 11% 10%</div> </div>
1	F	887	<div> <div>53%</div> <div>81% 8% 10%</div> </div>
1	G	887	<div> <div>44%</div> <div>81% 9% 10%</div> </div>
1	H	887	<div> <div>42%</div> <div>78% 12% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	887	<div><div>50%</div><div><div></div><div></div><div></div><div></div></div><div>79%</div><div>11%</div><div>10%</div></div>
1	J	887	<div><div>55%</div><div><div></div><div></div><div></div><div></div></div><div>78%</div><div>13%</div><div>8%</div></div>
2	P	1088	<div><div>53%</div><div><div></div><div></div><div></div><div></div></div><div>87%</div><div>13%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 148557 atoms, of which 74462 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	781	Total	C	H	N	O	S	0	0
			12787	4052	6408	1101	1190	36		
1	B	781	Total	C	H	N	O	S	0	0
			12787	4052	6408	1101	1190	36		
1	C	780	Total	C	H	N	O	S	0	0
			12772	4047	6400	1100	1189	36		
1	D	827	Total	C	H	N	O	S	0	0
			13574	4297	6809	1163	1269	36		
1	E	795	Total	C	H	N	O	S	0	0
			13028	4132	6529	1118	1213	36		
1	F	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	G	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	H	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	I	800	Total	C	H	N	O	S	0	0
			13114	4159	6569	1127	1223	36		
1	J	816	Total	C	H	N	O	S	0	0
			13391	4242	6713	1149	1251	36		

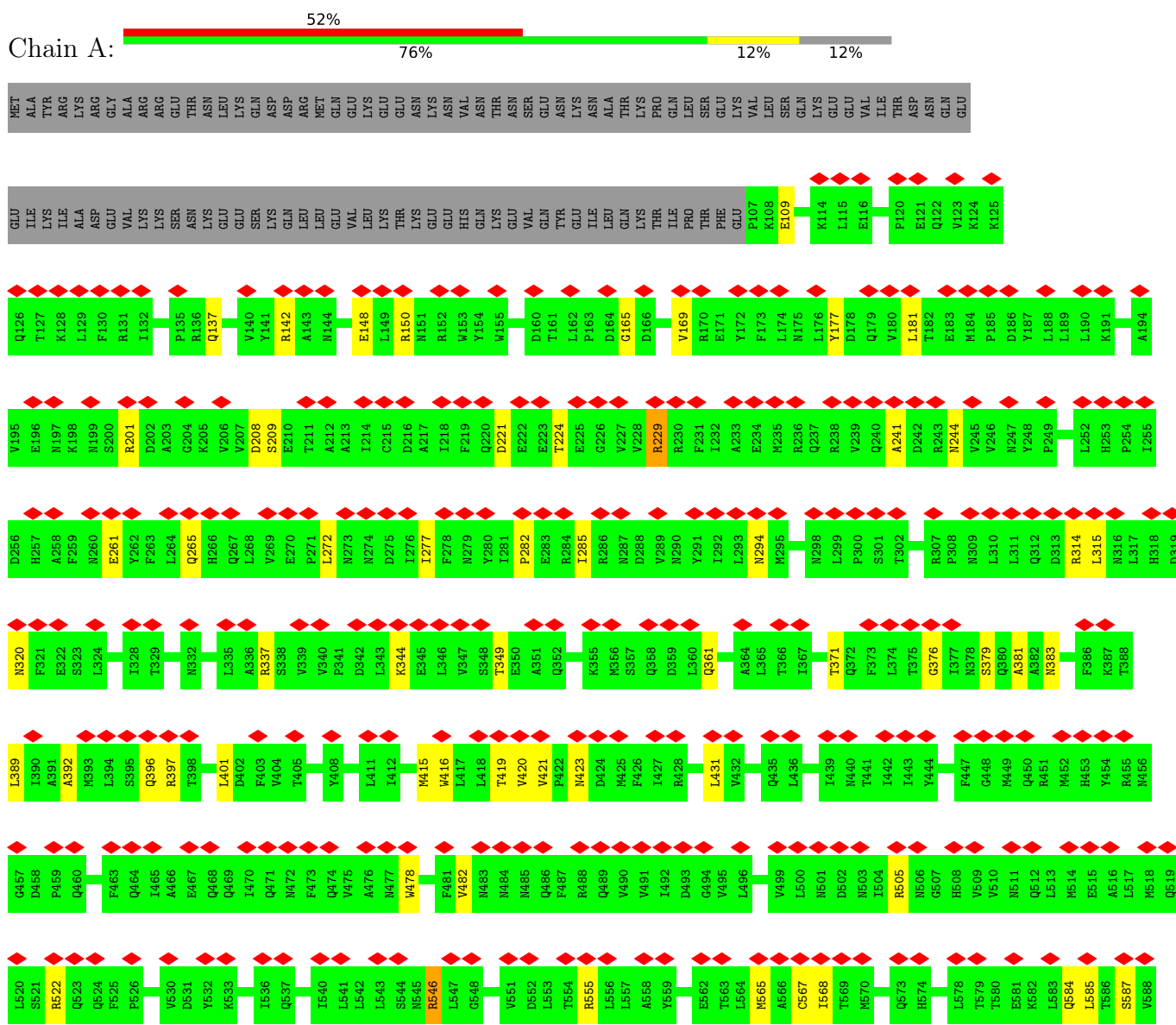
- Molecule 2 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	1086	Total	C	H	N	O	S	0	0
			17651	5633	8862	1455	1662	39		

3 Residue-property plots

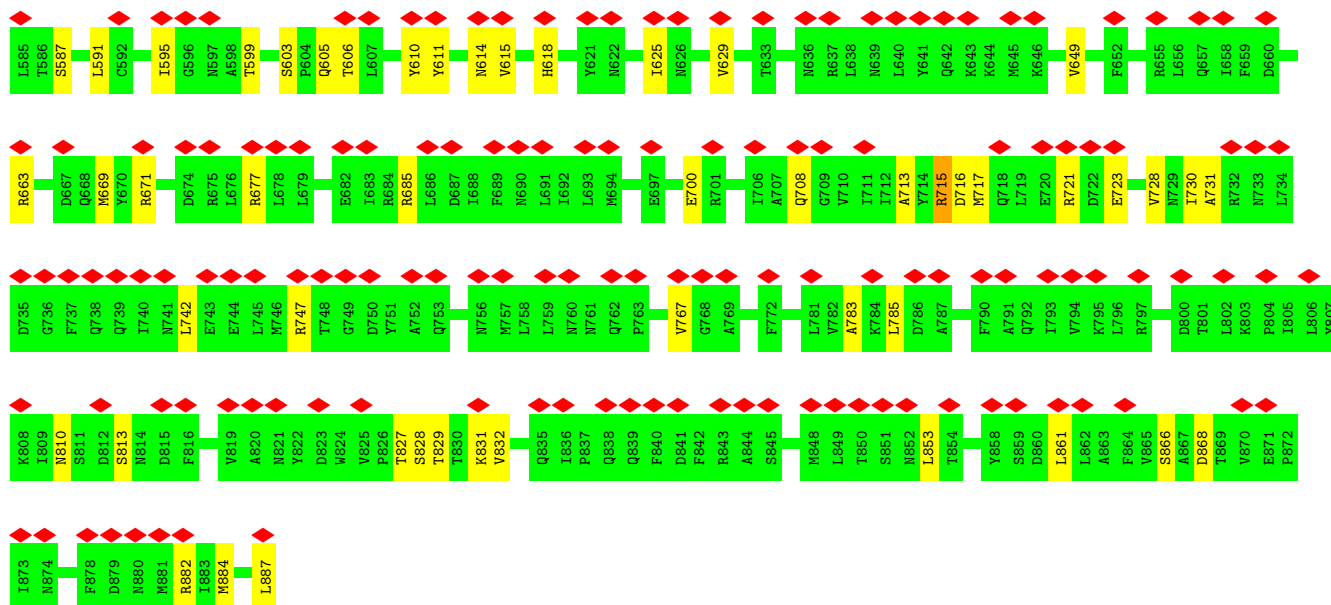
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Inner capsid protein VP2

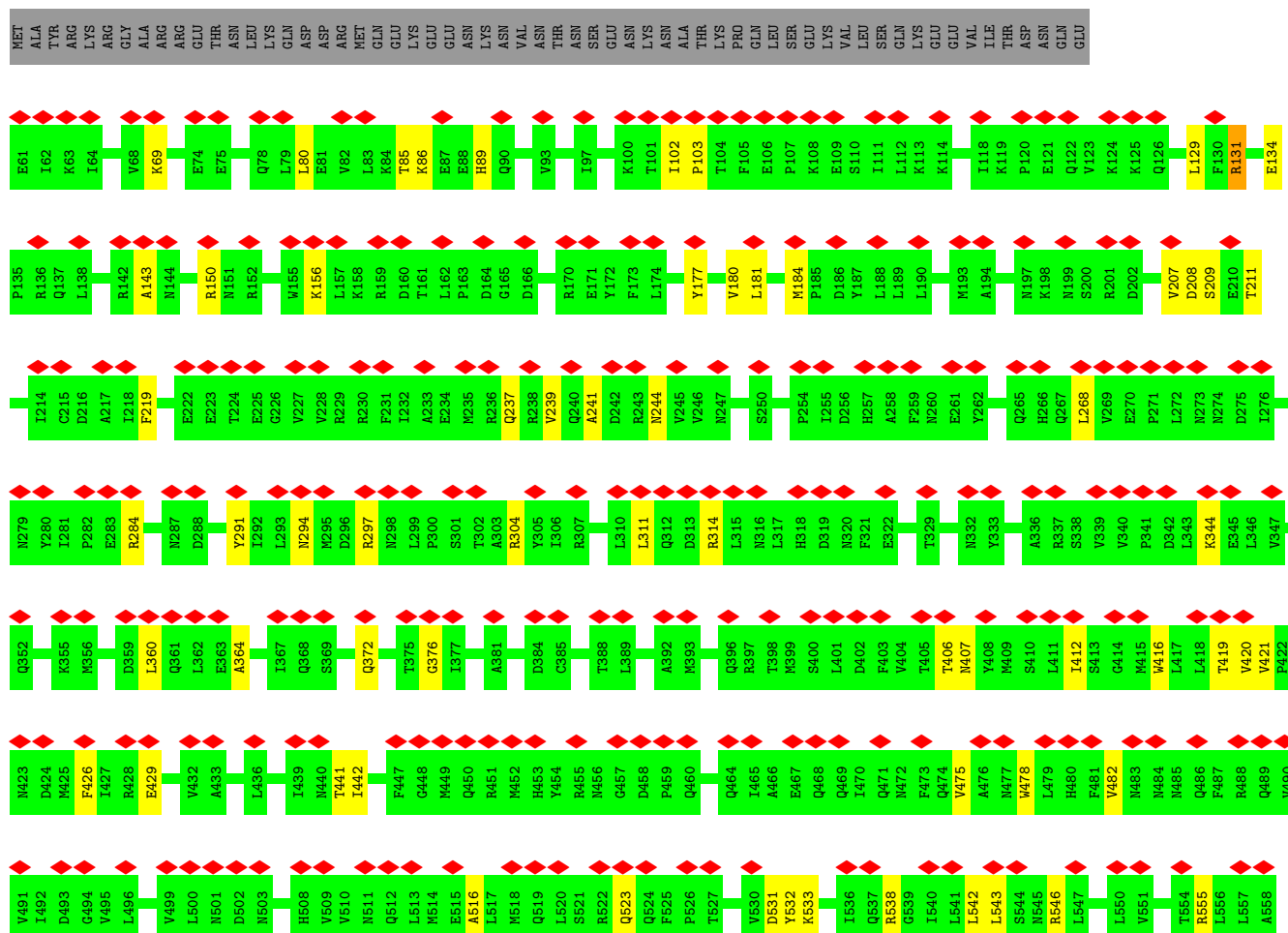
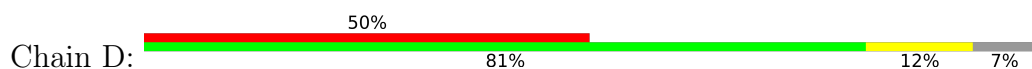


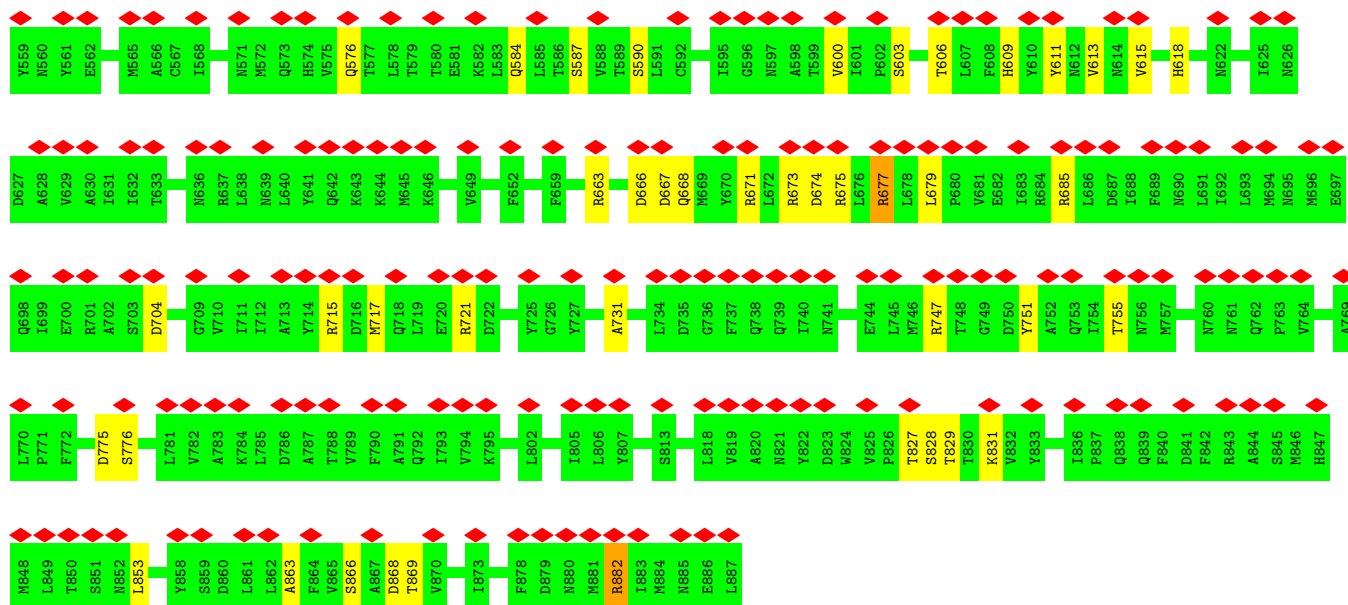


V482	N483	N484	N485	Q486	F487	R488	V491	L492	G494	N497	Q498	V499	N501	D502	N503	I504	R505	N506	G507	H508	V509	V510	N511	Q512	L513	M514	E515	A516	L517	M518	Q519	R522	Q523	Q524	F525	F526	T527	M528	F529	V530	D531	F532	K533	R534	S535	I536	Q537	R538	G539	I540	L541	S544		
I412	S413	G414	M415	M416	L417	L418	T419	W420	D424	M425	F426	I427	R428	L431	V432	L436	A437	I438	T441	I442	I443	A446	F447	G448	M449	Q450	R451	M452	H453	Y454	R455	P459	Q460	F463	Q464	A466	E467	Q468	Q469	I470	Q471	M472	F473	Q474	W475	A476	M477	W478	F481					
V339	V340	F341	D342	L343	K344	E345	L346	V347	S348	A351	Q352	I353	Q354	K355	M356	S357	Q358	D359	L360	Q361	L362	E363	A364	L365	T366	S369	E370	T371	Q372	F373	I377	M378	S379	A382	F386	T390	M393	L394	S395	Q396	R397	T398	L401	D402	F403	V404	T405	T406	M407	Y408	M409			
E270	P271	L272	M273	M274	D275	I276	I277	F278	M279	E283	R284	I285	R286	M287	D288	V289	M290	Y291	I292	L293	M294	R295	D296	R297	M298	L299	P300	S301	T302	A303	R307	P308	M309	L310	L311	Q312	D313	R314	L315	M316	L317	H318	D319	M320	F321	E322	I328	T329	M332	Y333	I334	L335	A336	R337
A203	G204	V207	D208	S209	E210	T211	A212	I214	C215	D216	A217	I218	Q220	D221	E222	E223	T224	E225	Q226	V227	V228	R229	R230	F231	I232	A233	E234	M235	R236	Q237	R238	V239	Q240	A241	D242	R243	N244	M247	L252	H253	P254	I255	D256	H257	A258	E261	L264	Q265	H266	Q267	L268	P269		
Q122	V123	K124	K125	Q126	T127	K128	L129	F130	R131	I132	F133	E134	P135	V140	Y141	R142	A143	M144	E148	L149	R150	M151	R152	M153	Y154	W155	K158	R159	D160	G165	D166	V169	R170	F173	L176	Y177	V180	L181	Y187	L188	L189	L190	K191	A194	M197	R201	D202							
GLU	ILE	LYS	ILE	ALA	ASP	GLU	VAL	ALA	LYS	ARG	LYS	ARG	THR	ASN	LYS	GLU	VAL	LYS	THR	LYS	GLU	GLN	VAL	GLN	TYR	GLU	ILE	LEU	GLN	LYS	THR	PRO	ILE	THR	PHE	GLU	P107	K108	E109	L112	K113	K114	L115	E116	D117	I118	K119	P120	E121					
MET	ALA	TYR	ARG	LYS	ARG	GLY	ALA	ARG	ARG	THR	ASN	LYS	ASN	LEU	LYS	GLN	LEU	LEU	MET	GLN	GLU	LYS	GLU	GLN	ASN	LYS	ASN	ALA	THR	LYS	PRO	GLN	LEU	SER	GLN	GLU	GLU	VAL	ILE	THR	ASP	ASN	GLN	GLU										

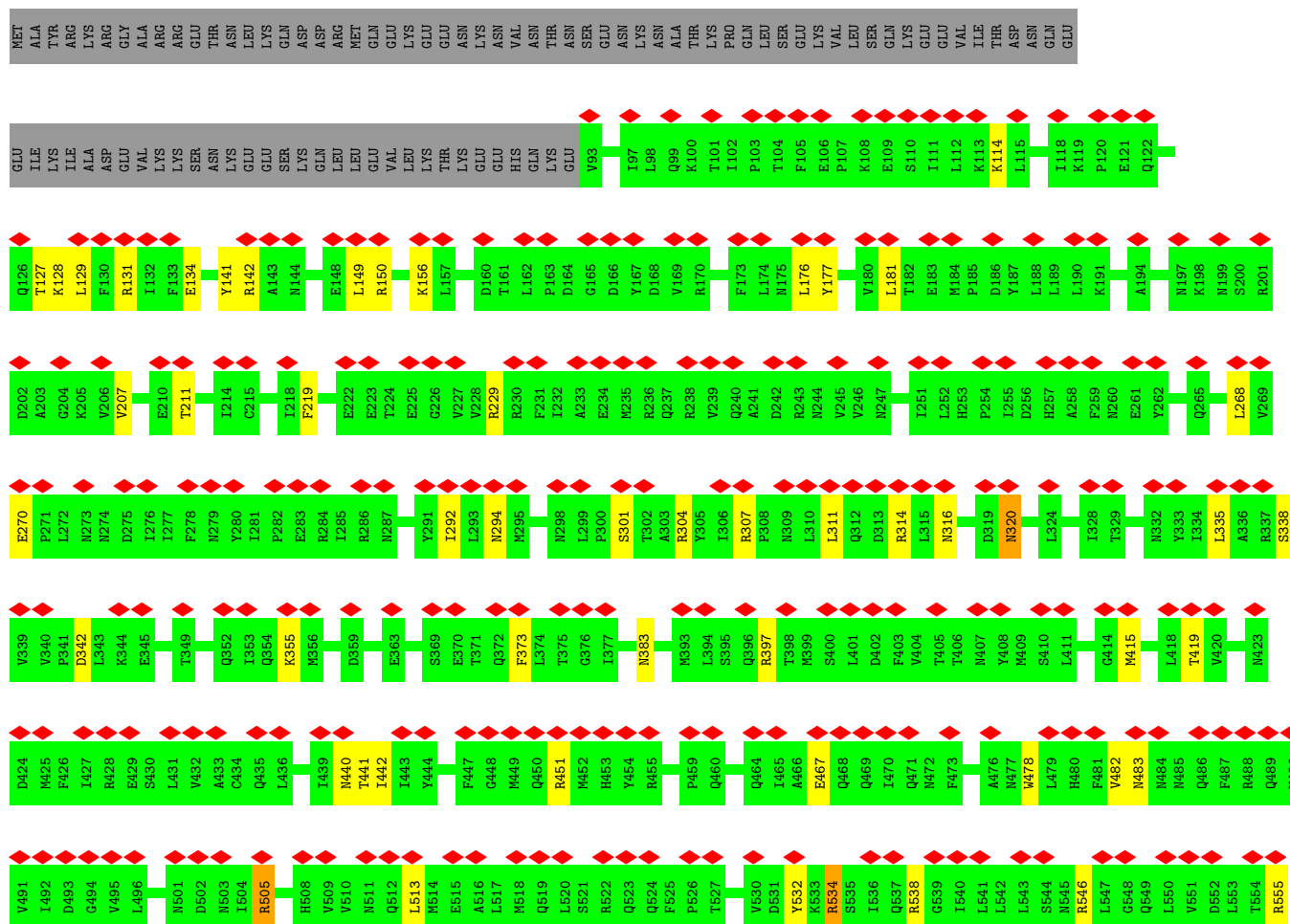
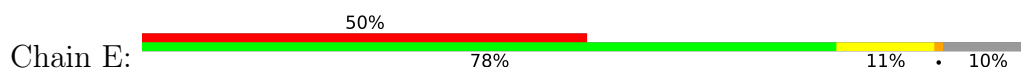


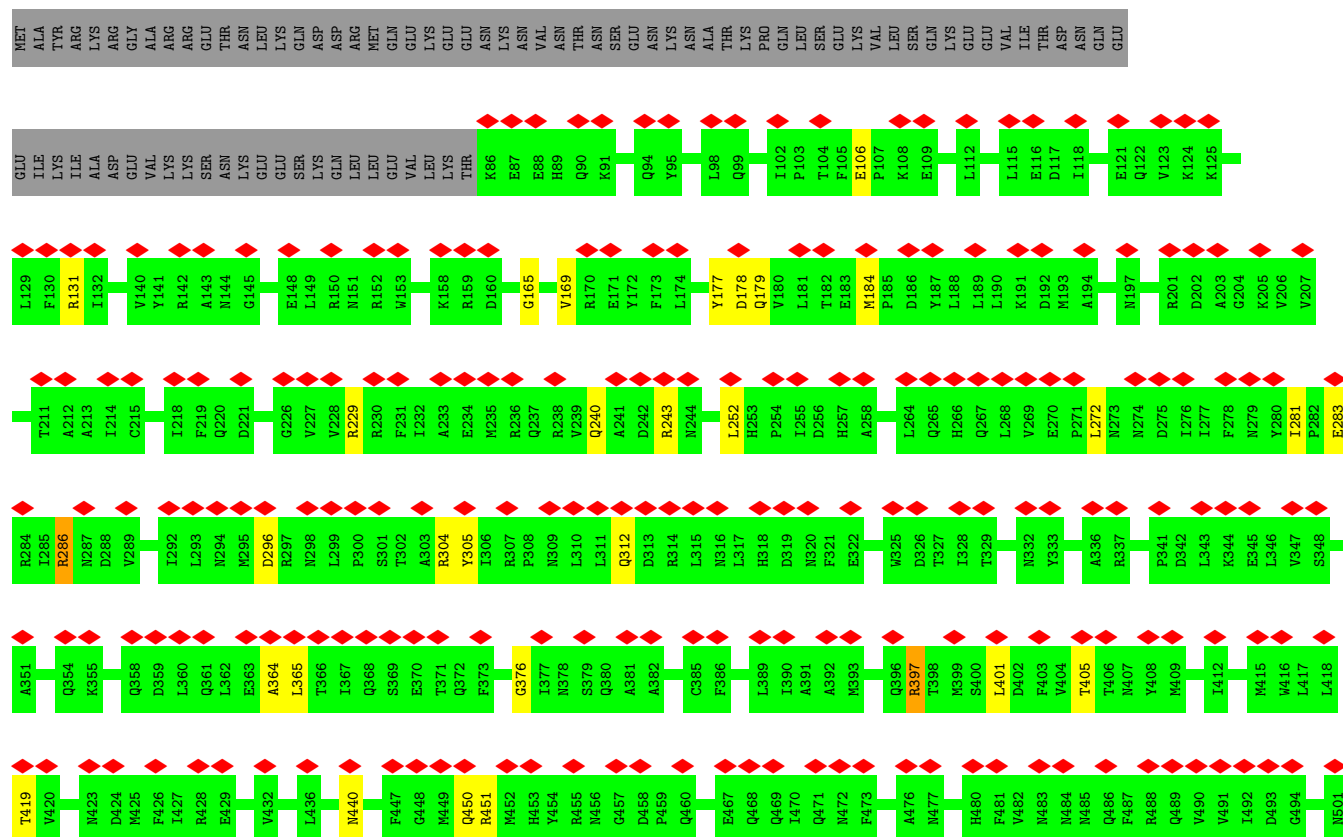
• Molecule 1: Inner capsid protein VP2

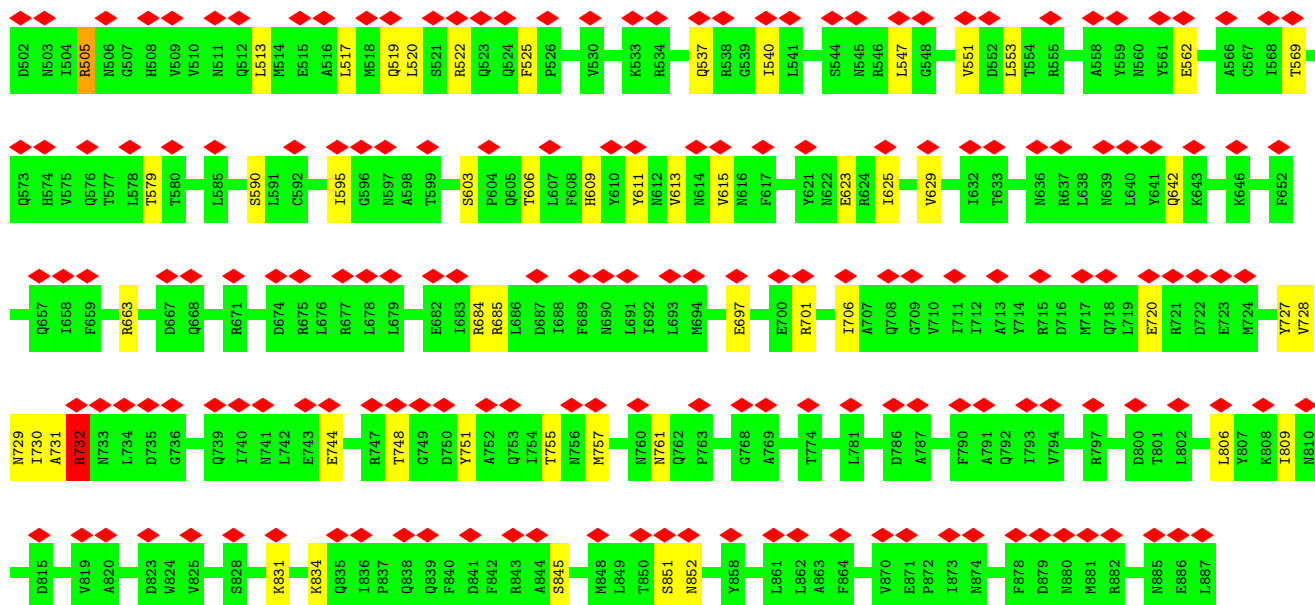




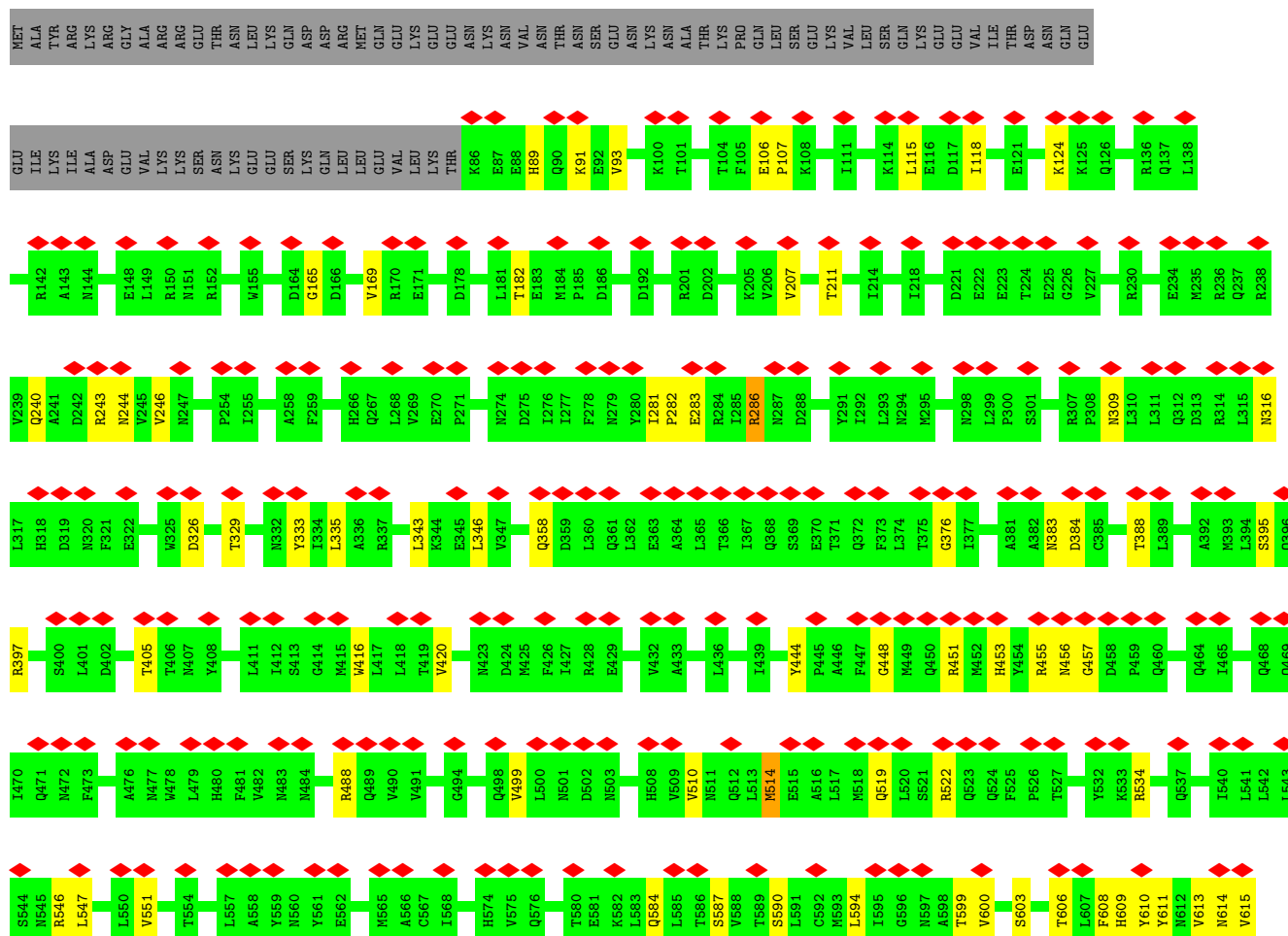
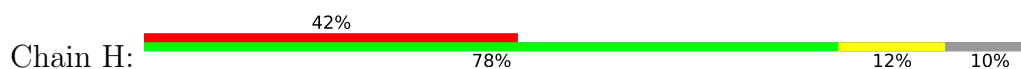
• Molecule 1: Inner capsid protein VP2

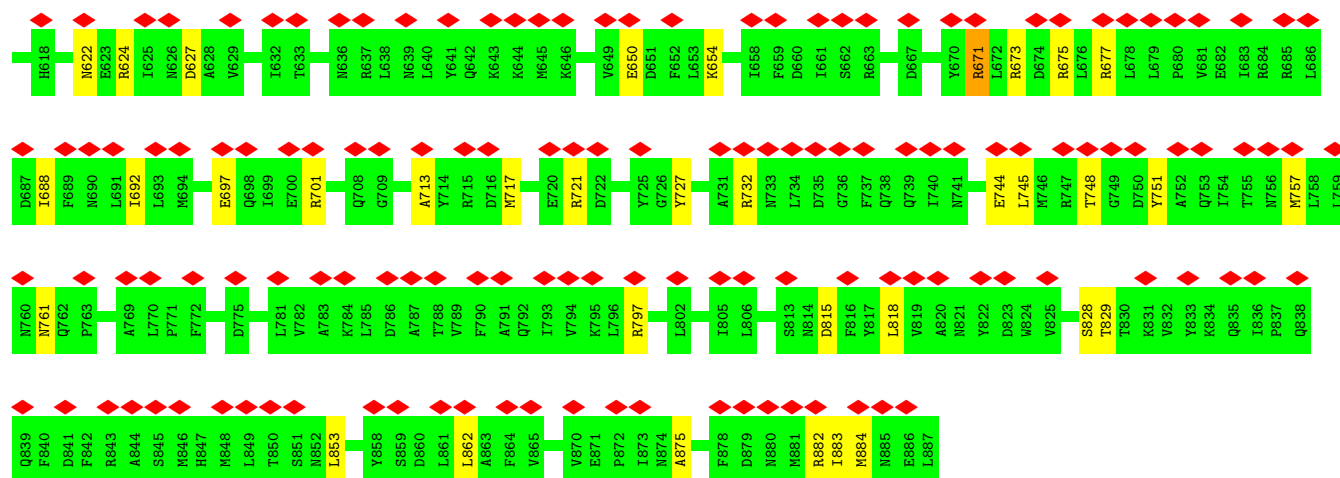




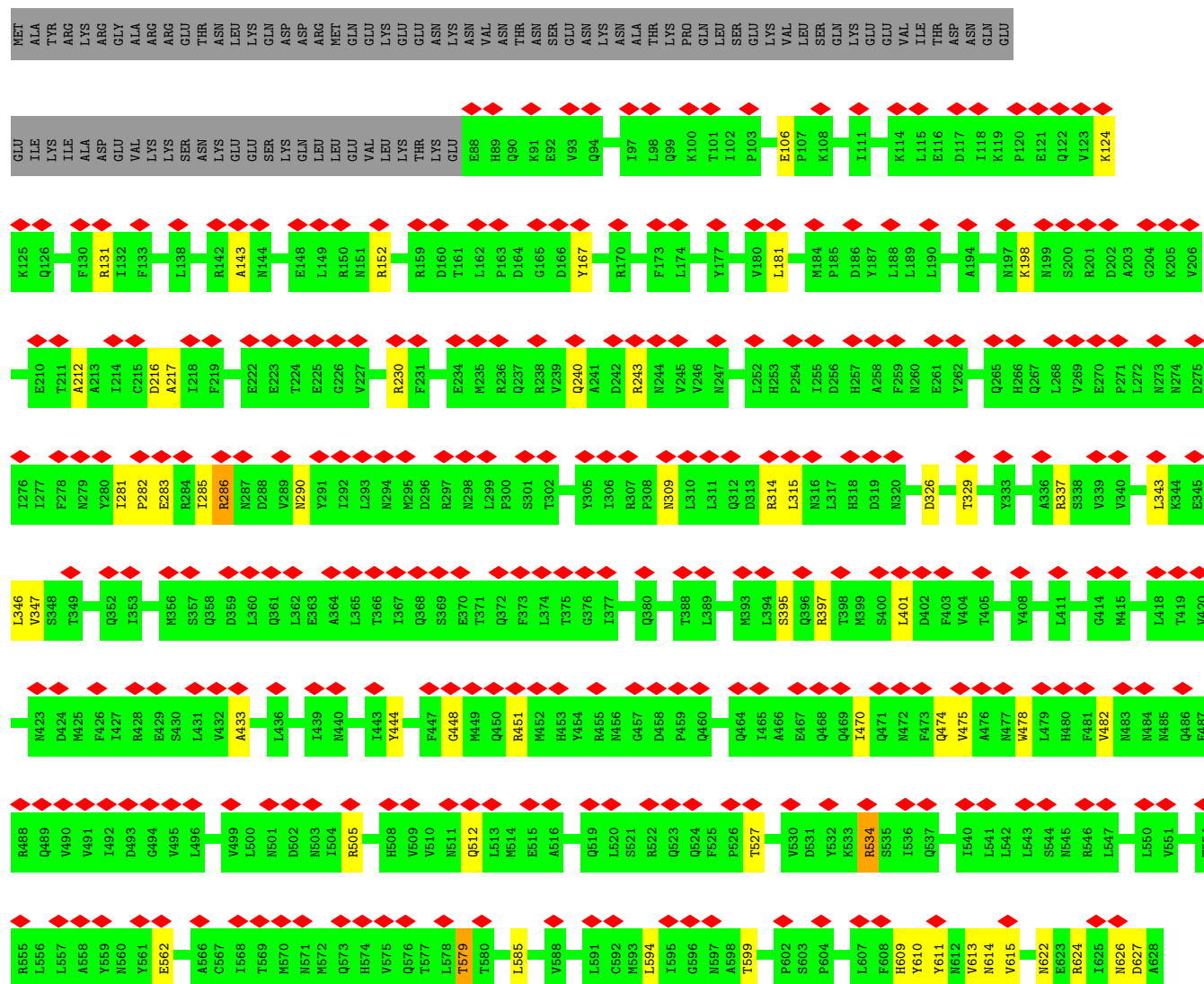
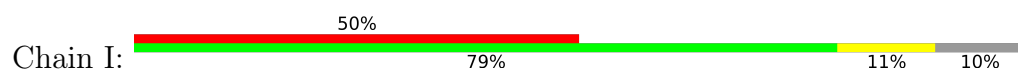


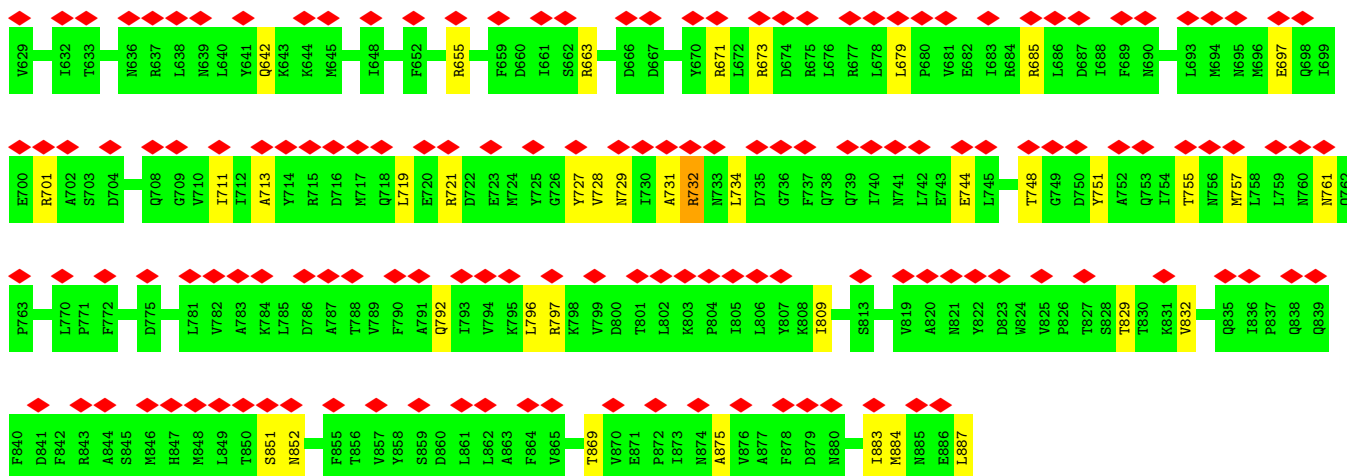
• Molecule 1: Inner capsid protein VP2



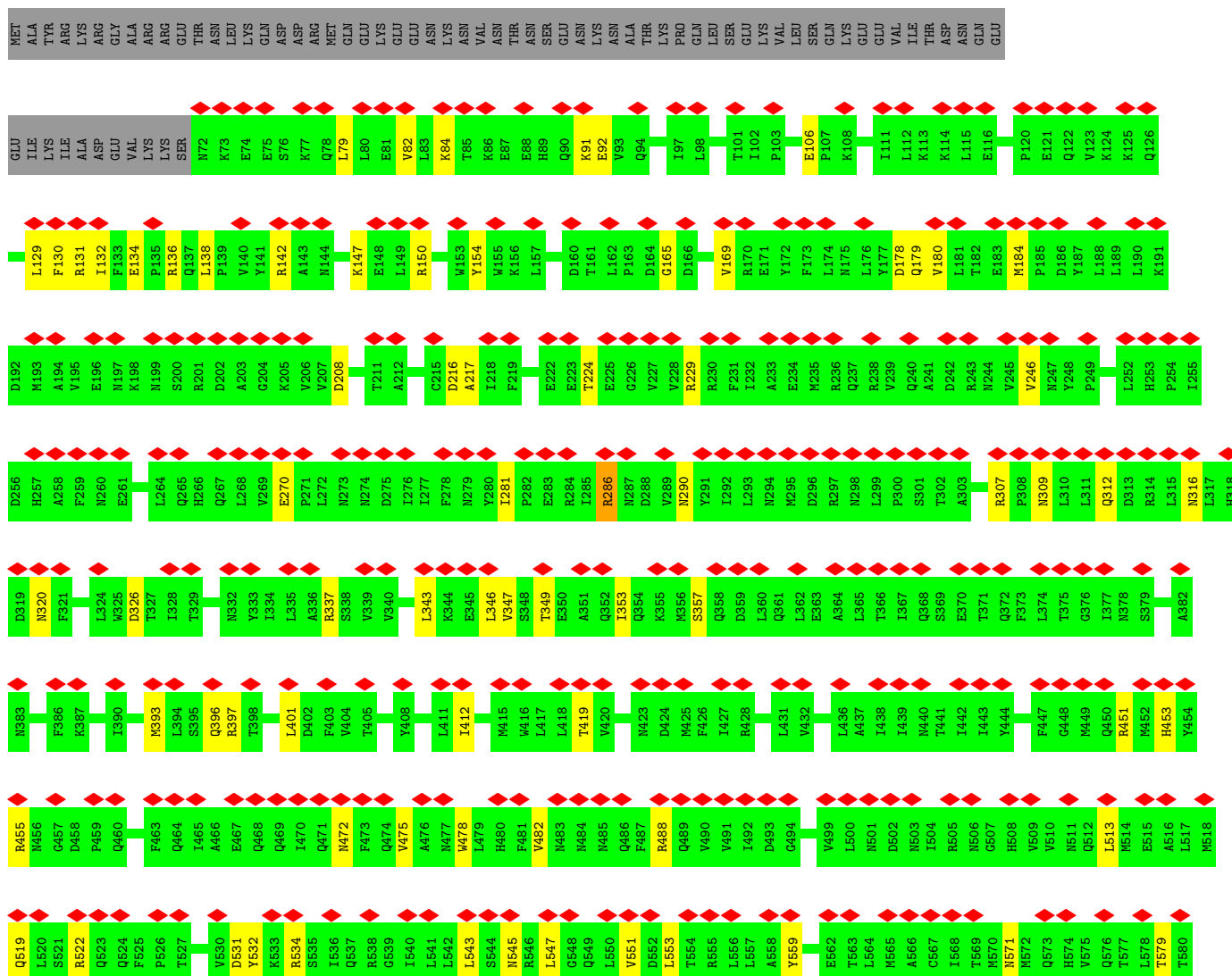
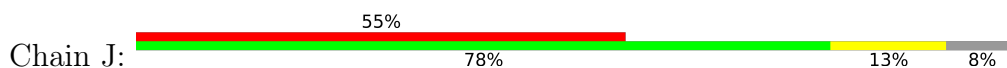


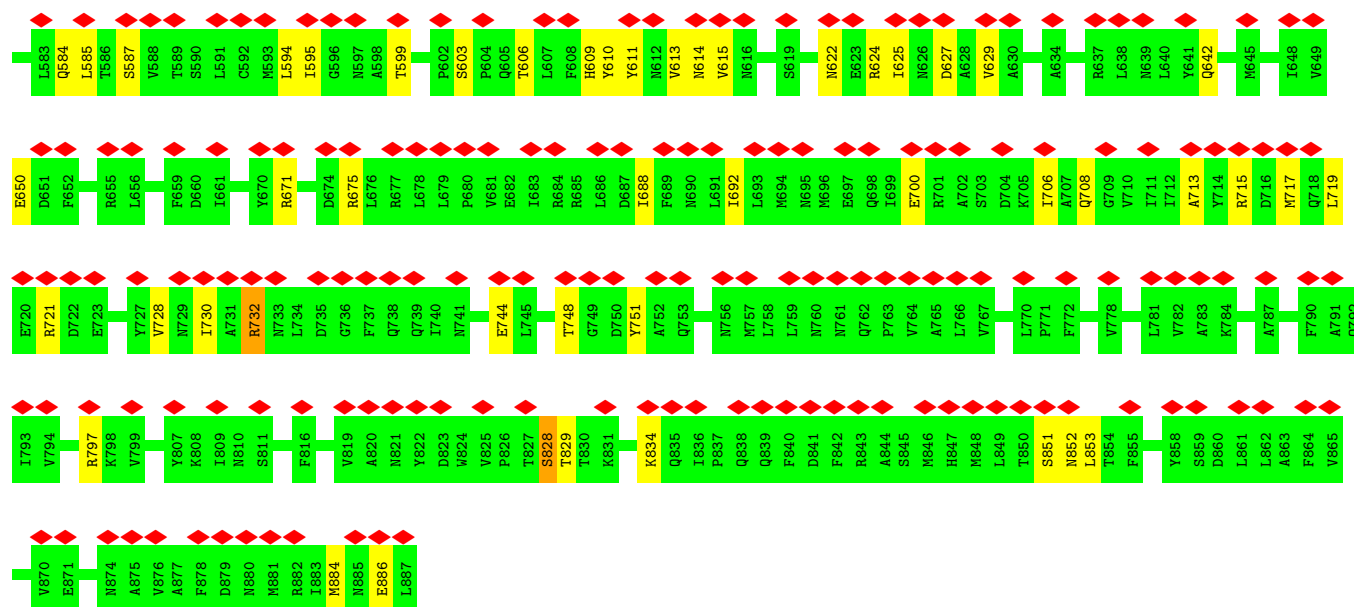
• Molecule 1: Inner capsid protein VP2



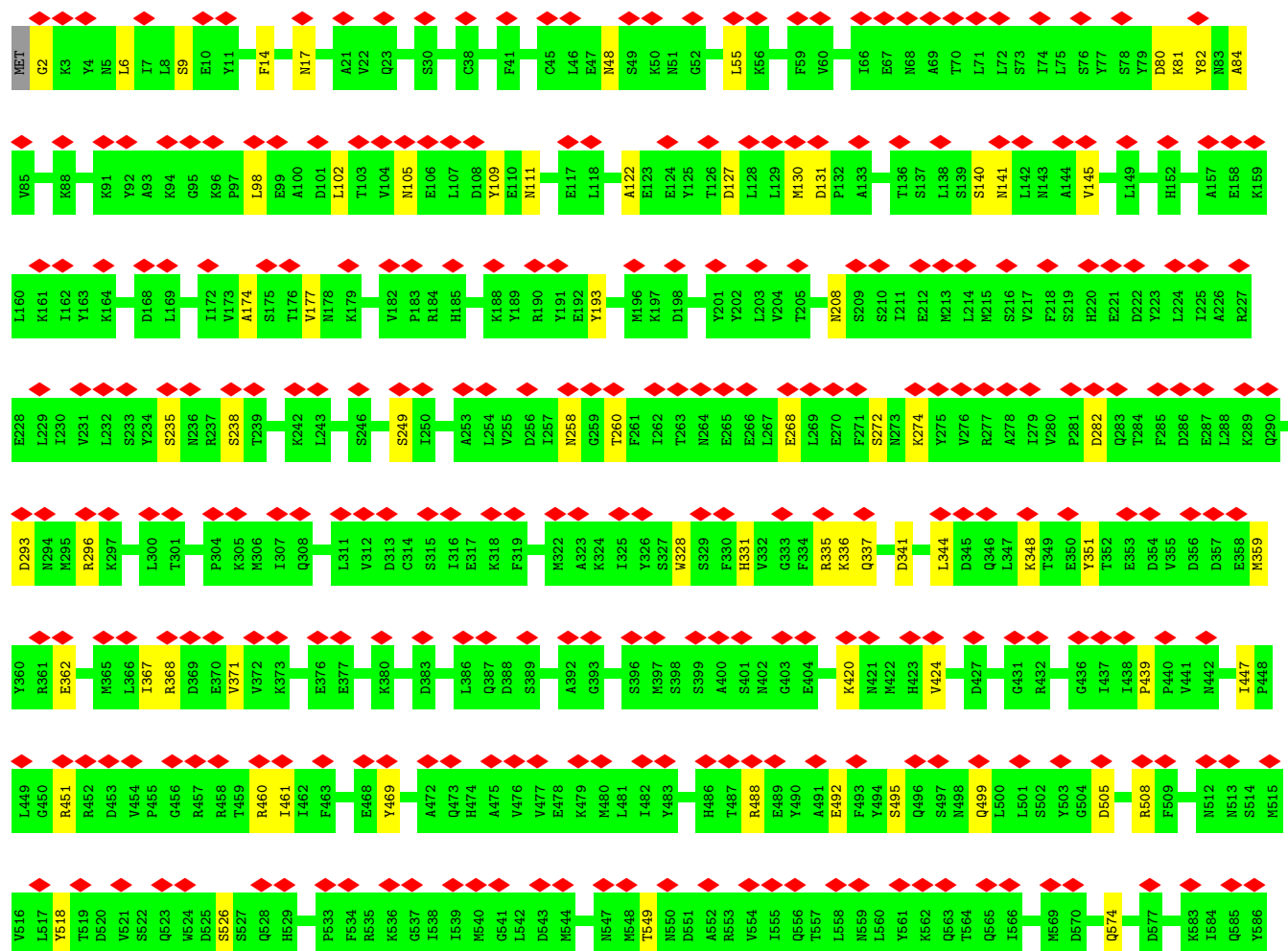
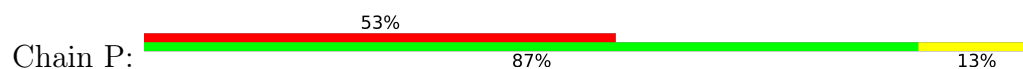


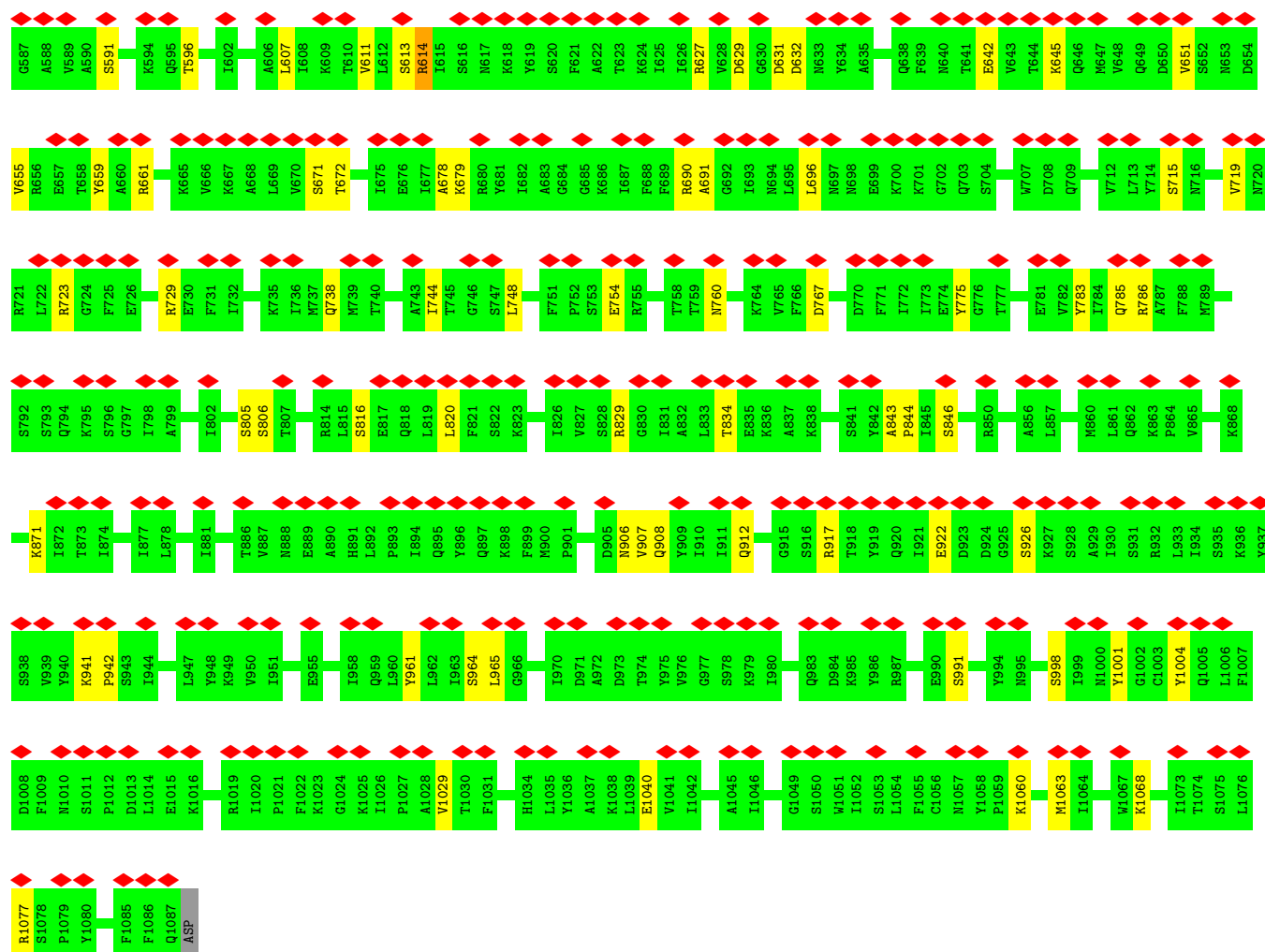
• Molecule 1: Inner capsid protein VP2





• Molecule 2: RNA-directed RNA polymerase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.245	Depositor
Minimum map value	-6.056	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.486	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	369.0, 369.0, 369.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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	0.50	0/6495	0.91	16/8810 (0.2%)
1	B	0.48	0/6495	0.90	18/8810 (0.2%)
1	C	0.49	1/6487 (0.0%)	0.90	15/8799 (0.2%)
1	D	0.48	0/6885	0.89	15/9332 (0.2%)
1	E	0.49	0/6618	0.91	16/8979 (0.2%)
1	F	0.48	0/6683	0.88	12/9064 (0.1%)
1	G	0.47	0/6683	0.86	9/9064 (0.1%)
1	H	0.48	0/6683	0.88	8/9064 (0.1%)
1	I	0.48	0/6665	0.87	14/9041 (0.2%)
1	J	0.48	0/6798	0.87	9/9217 (0.1%)
2	P	0.48	0/8963	0.85	8/12120 (0.1%)
All	All	0.48	1/75455 (0.0%)	0.88	140/102300 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	F	0	1
1	G	0	3
1	H	0	1
1	I	0	3
1	J	0	3
2	P	0	2
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	ILE	C-N	-5.05	1.22	1.34

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	882	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	C	671	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	671	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	D	882	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	G	397	ARG	NE-CZ-NH2	-7.10	116.75	120.30

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	371	THR	Peptide
1	B	143	ALA	Peptide
1	C	143	ALA	Peptide
1	D	102	ILE	Peptide
1	D	143	ALA	Peptide

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	6379	6408	6408	56	0
1	B	6379	6408	6408	62	0
1	C	6372	6400	6399	63	0
1	D	6765	6809	6809	57	0
1	E	6499	6529	6529	59	0
1	F	6563	6588	6588	50	0
1	G	6563	6588	6588	44	0
1	H	6563	6588	6588	59	0
1	I	6545	6569	6569	50	0
1	J	6678	6713	6713	67	0
2	P	8789	8862	8861	77	0
All	All	74095	74462	74460	597	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 597 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)
2:P:359:MET:SD	2:P:614:ARG:NH2	2.61	0.73
1:F:744:GLU:O	1:F:748:THR:OG1	2.06	0.72
1:G:281:ILE:O	1:G:286:ARG:NH1	2.23	0.72
1:F:281:ILE:O	1:F:286:ARG:NH1	2.23	0.71
1:F:309:ASN:O	1:F:622:ASN:ND2	2.23	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/887 (88%)	712 (91%)	67 (9%)	0	100	100
1	B	779/887 (88%)	714 (92%)	65 (8%)	0	100	100
1	C	778/887 (88%)	706 (91%)	72 (9%)	0	100	100
1	D	825/887 (93%)	752 (91%)	72 (9%)	1 (0%)	51	85
1	E	793/887 (89%)	720 (91%)	73 (9%)	0	100	100
1	F	800/887 (90%)	720 (90%)	80 (10%)	0	100	100
1	G	800/887 (90%)	721 (90%)	79 (10%)	0	100	100
1	H	800/887 (90%)	722 (90%)	77 (10%)	1 (0%)	51	85
1	I	798/887 (90%)	724 (91%)	74 (9%)	0	100	100
1	J	814/887 (92%)	739 (91%)	75 (9%)	0	100	100
2	P	1084/1088 (100%)	985 (91%)	96 (9%)	3 (0%)	41	76
All	All	9050/9958 (91%)	8215 (91%)	830 (9%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	82	TYR
2	P	84	ALA
2	P	942	PRO
1	H	107	PRO
1	D	103	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	717/818 (88%)	715 (100%)	2 (0%)	92	95
1	B	717/818 (88%)	716 (100%)	1 (0%)	93	97
1	C	716/818 (88%)	716 (100%)	0	100	100
1	D	762/818 (93%)	762 (100%)	0	100	100
1	E	731/818 (89%)	729 (100%)	2 (0%)	92	95
1	F	738/818 (90%)	737 (100%)	1 (0%)	93	97
1	G	738/818 (90%)	737 (100%)	1 (0%)	93	97
1	H	738/818 (90%)	737 (100%)	1 (0%)	93	97
1	I	736/818 (90%)	735 (100%)	1 (0%)	93	97
1	J	752/818 (92%)	751 (100%)	1 (0%)	93	97
2	P	986/989 (100%)	985 (100%)	1 (0%)	93	97
All	All	8331/9169 (91%)	8320 (100%)	11 (0%)	93	97

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	732	ARG
1	I	732	ARG
2	P	130	MET
1	J	732	ARG
1	E	320	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	622	ASN
1	H	549	GLN
2	P	785	GLN
1	J	614	ASN
1	J	636	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.

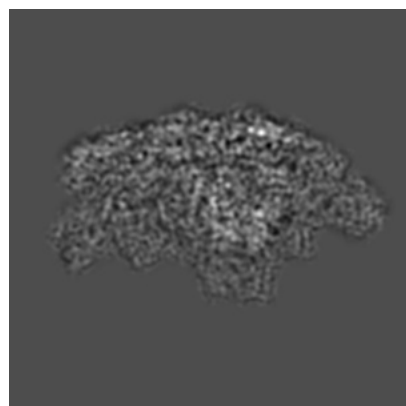
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20088. These allow visual inspection of the internal detail of the map and identification of artifacts.

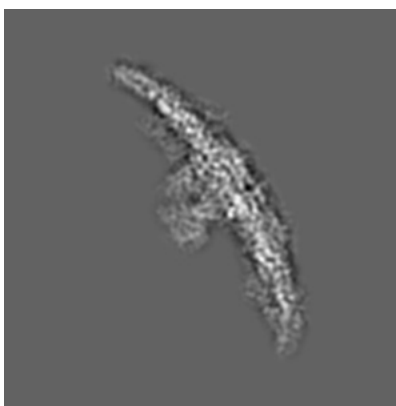
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

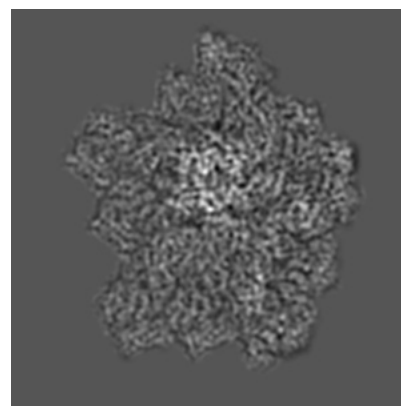
6.1.1 Primary map



X

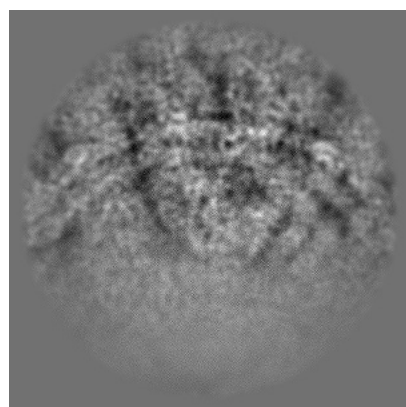


Y

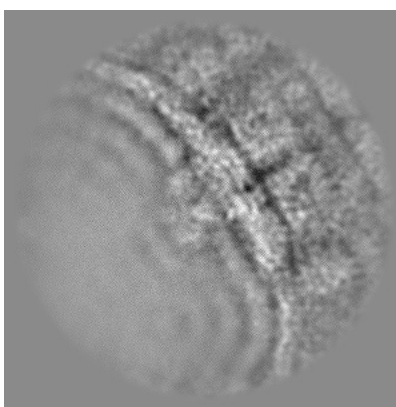


Z

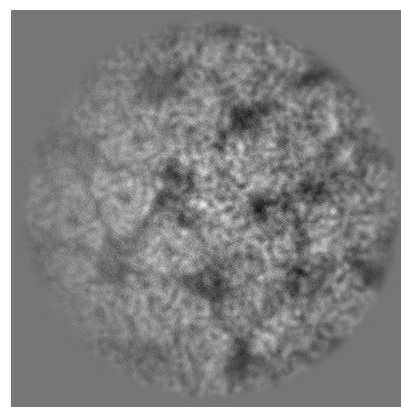
6.1.2 Raw map



X



Y



Z

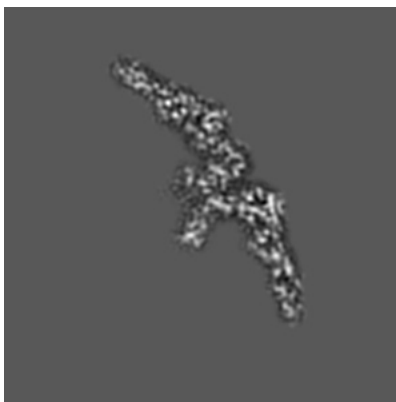
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150

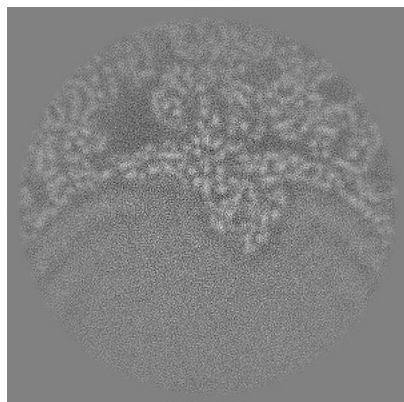


Y Index: 150

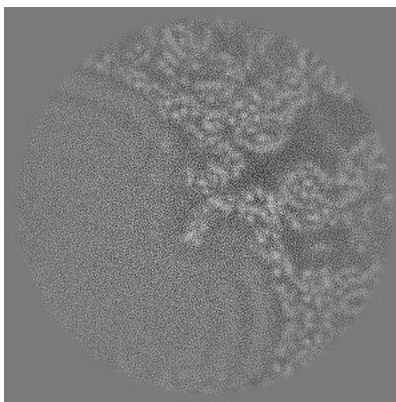


Z Index: 150

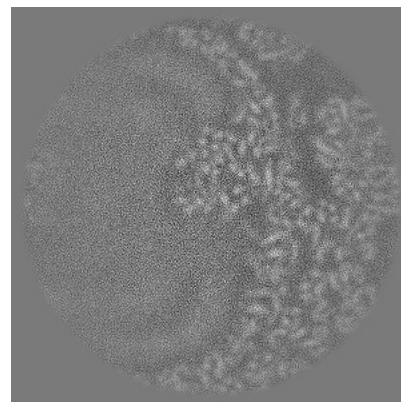
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

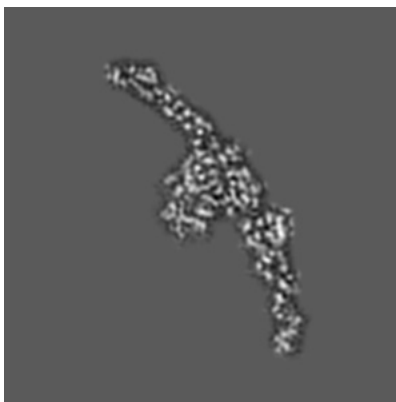
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 146

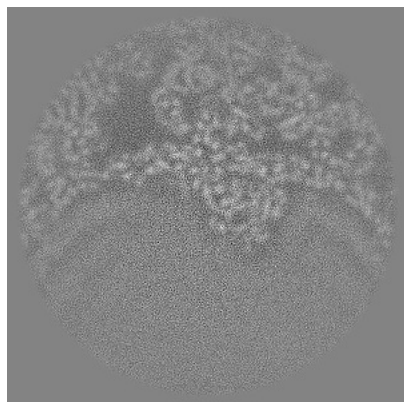


Y Index: 189

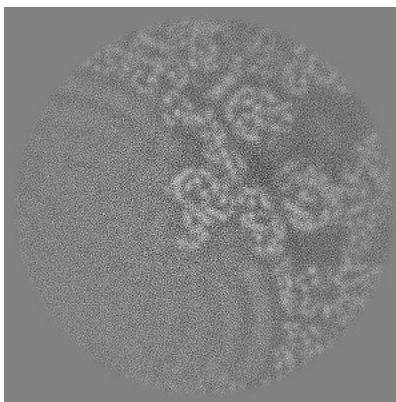


Z Index: 147

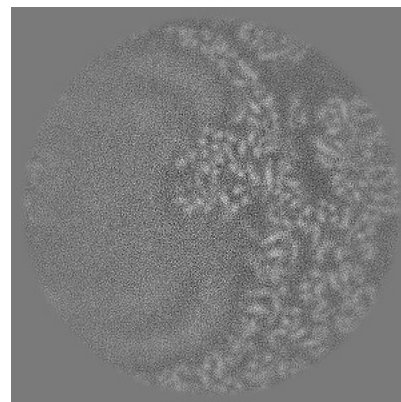
6.3.2 Raw map



X Index: 152



Y Index: 155

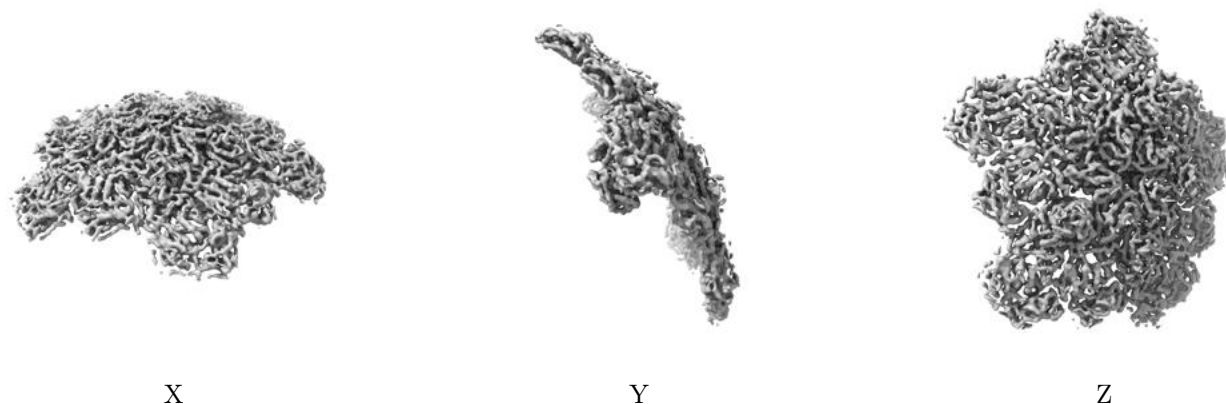


Z Index: 150

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

6.5 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

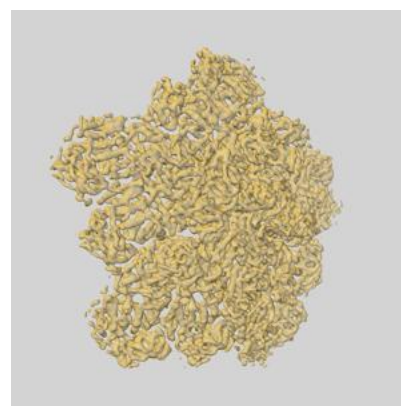
6.5.1 emd_20088_msk_1.map [i](#)



X



Y

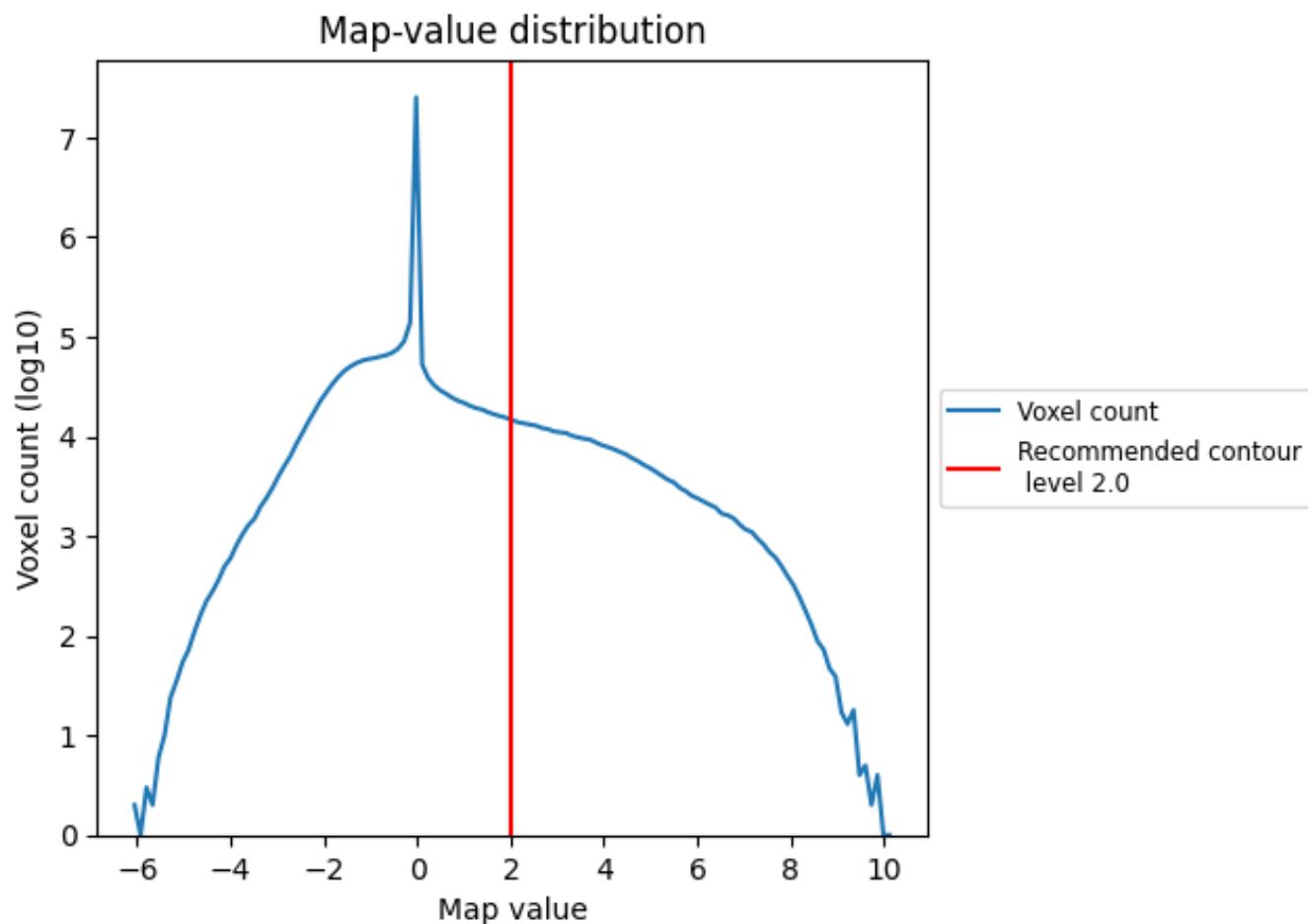


Z

7 Map analysis [i](#)

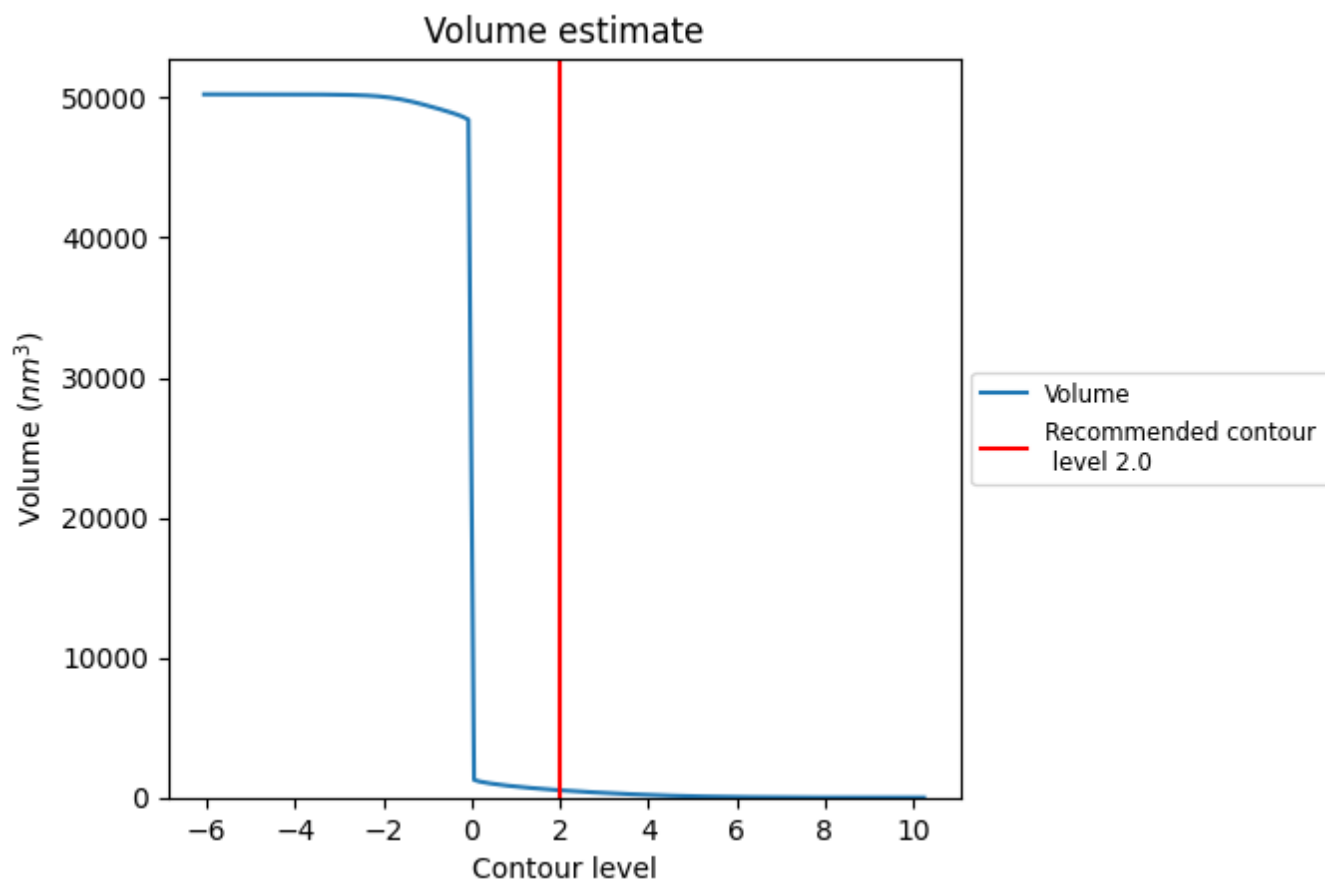
This section contains the results of statistical analysis of the map.

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.

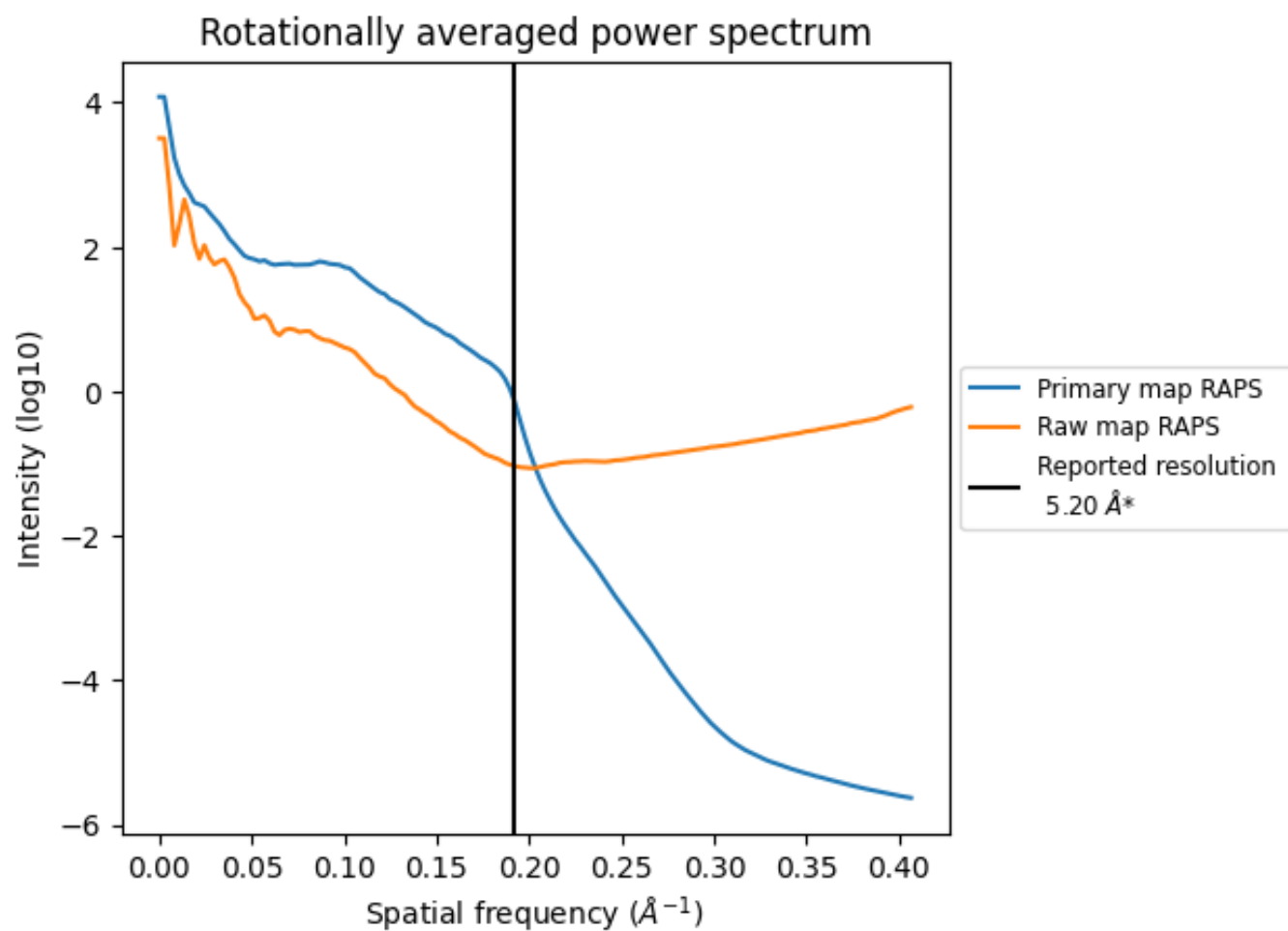
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 523 nm³; this corresponds to an approximate mass of 473 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 ⓘ

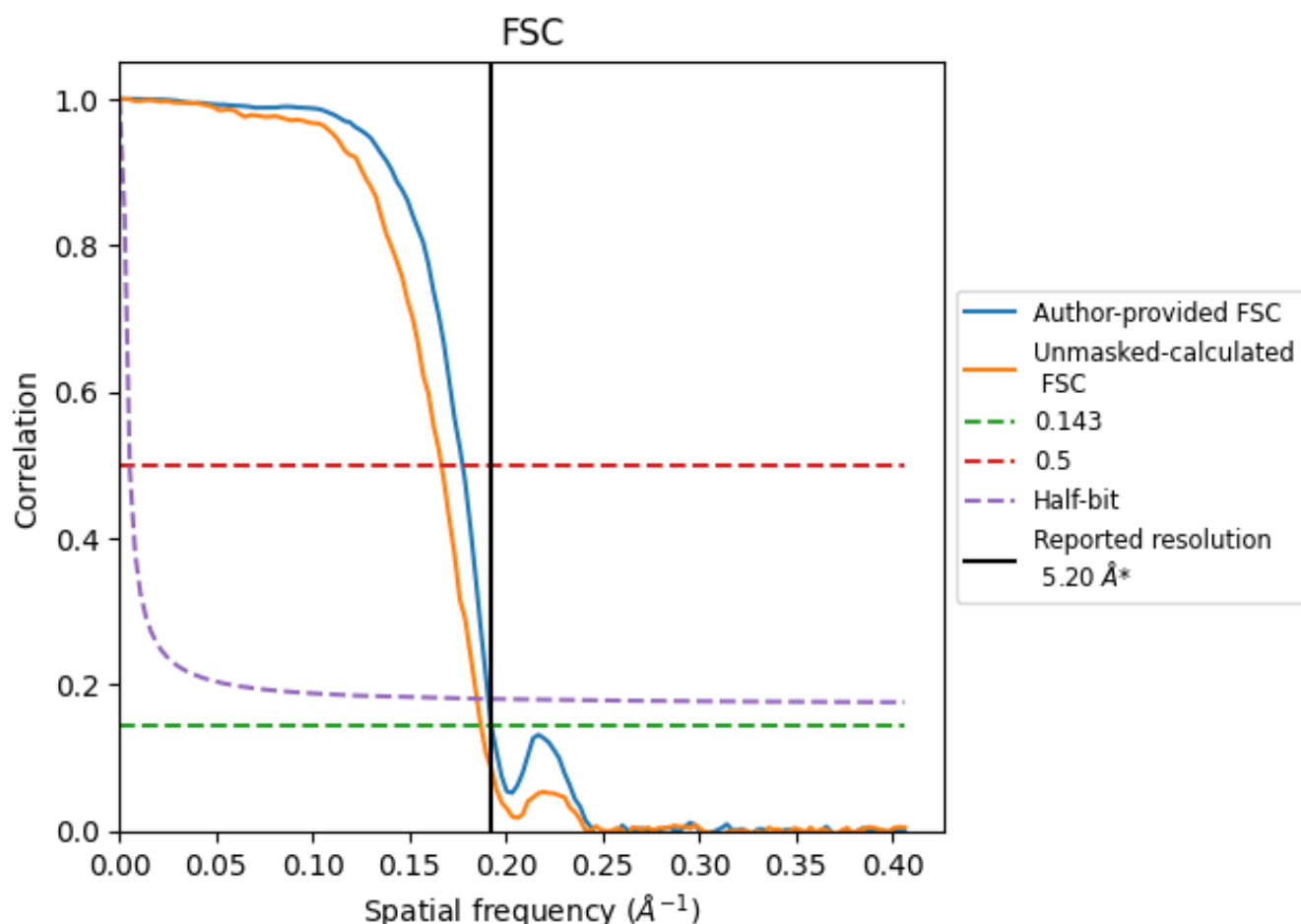


*Reported resolution corresponds to spatial frequency of 0.192 Å⁻¹

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 0.192 Å⁻¹

8.2 Resolution estimates [i](#)

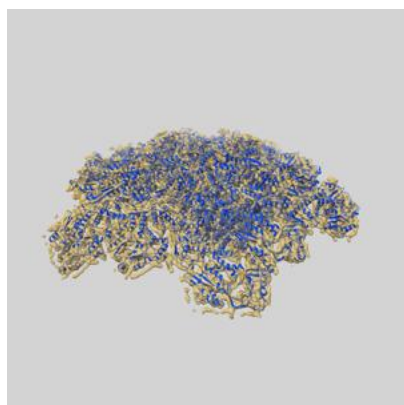
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	5.20	5.63	5.24
Unmasked-calculated*	5.34	6.00	5.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

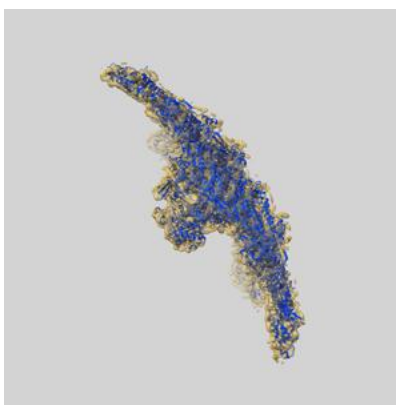
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20088 and PDB model 6OJ5. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

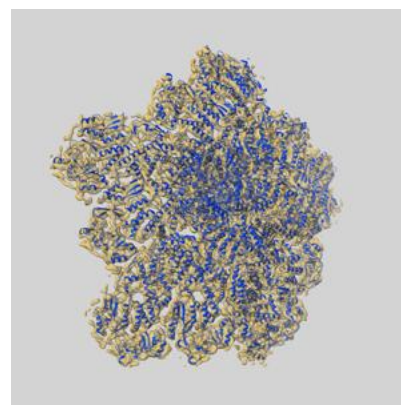
9.1 Map-model overlay [i](#)



X



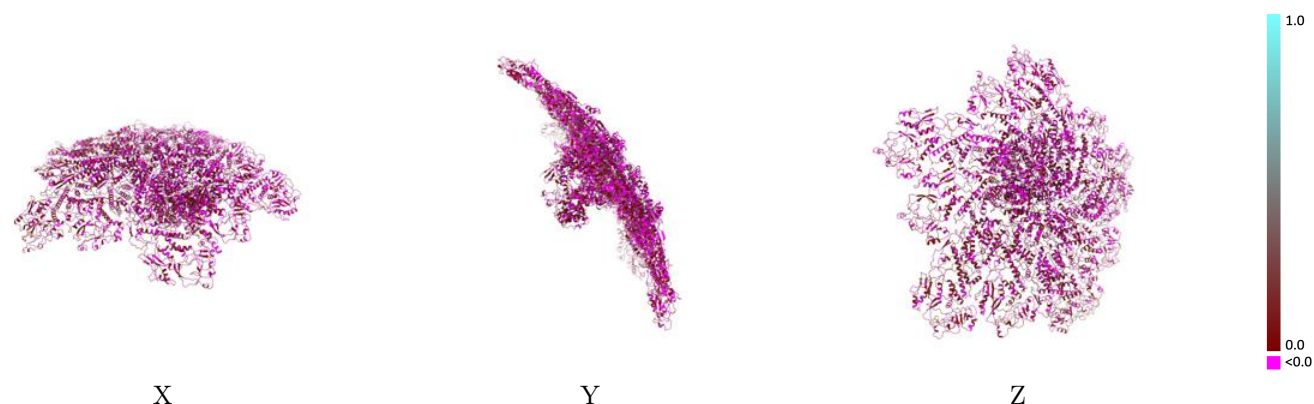
Y



Z

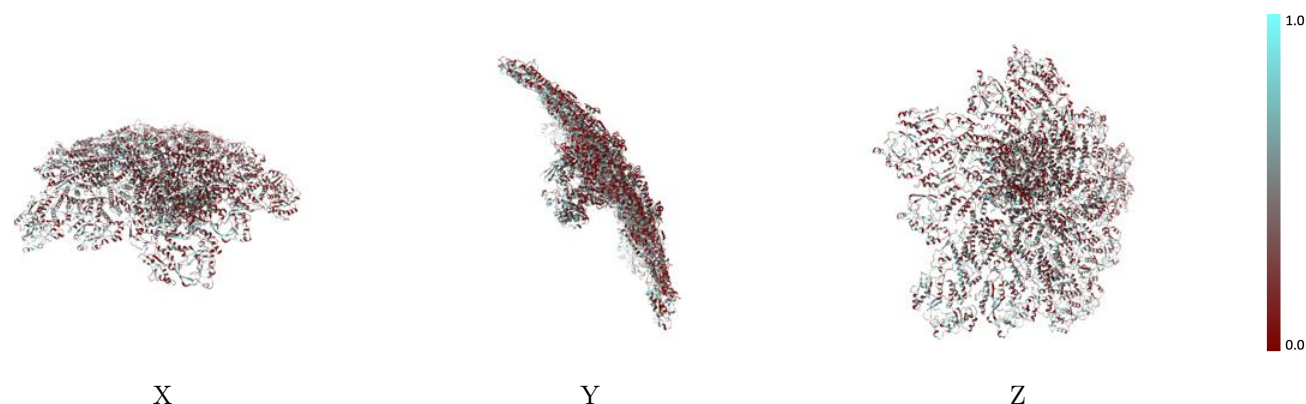
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



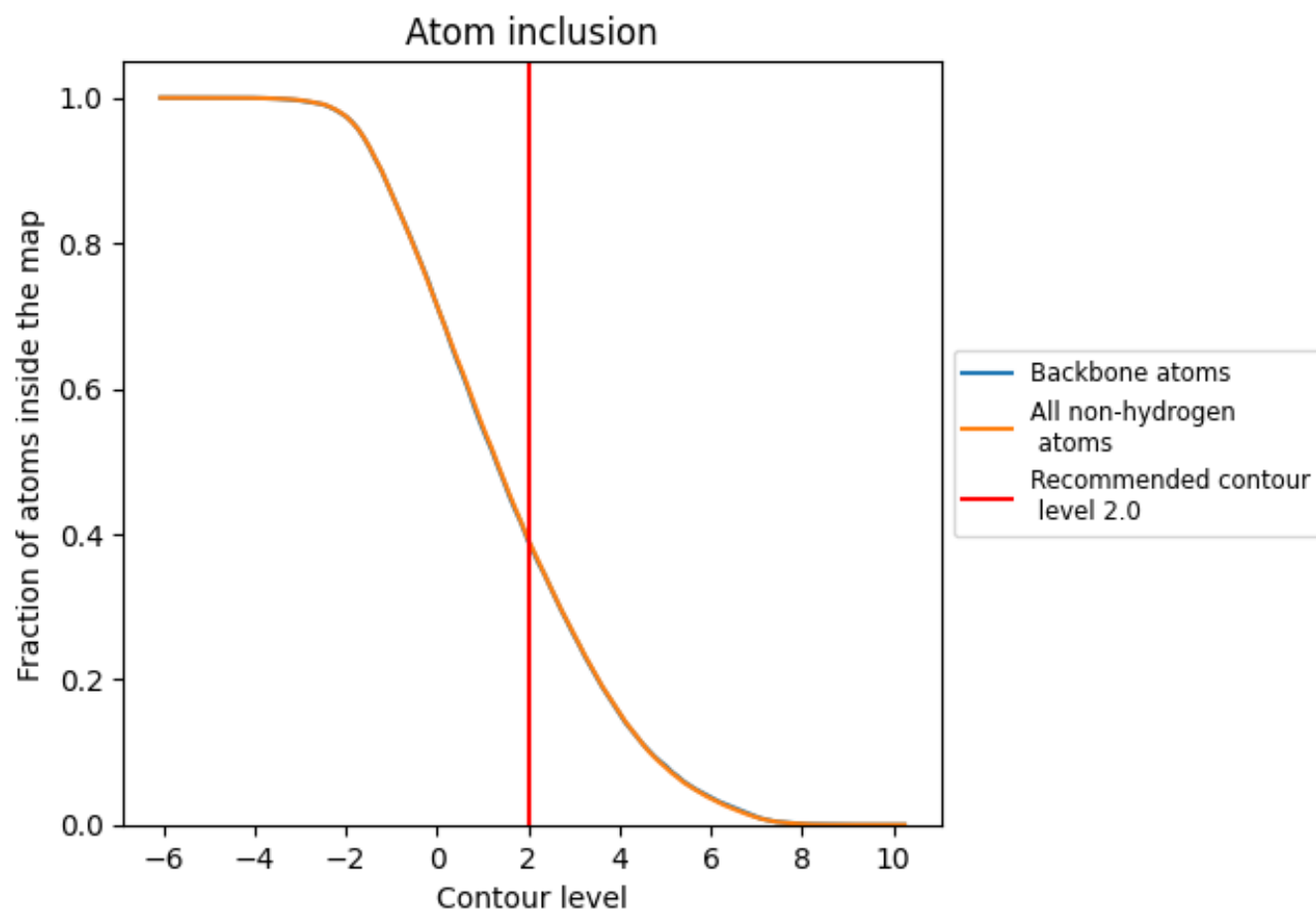
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 39% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3924	<div></div> 0.0760
A	<div></div> 0.3665	<div></div> 0.0520
B	<div></div> 0.4110	<div></div> 0.0810
C	<div></div> 0.4344	<div></div> 0.1090
D	<div></div> 0.4066	<div></div> 0.0890
E	<div></div> 0.3837	<div></div> 0.0650
F	<div></div> 0.3662	<div></div> 0.0470
G	<div></div> 0.4384	<div></div> 0.1050
H	<div></div> 0.4325	<div></div> 0.1090
I	<div></div> 0.3867	<div></div> 0.0660
J	<div></div> 0.3460	<div></div> 0.0360
P	<div></div> 0.4043	<div></div> 0.0770

