



# wwPDB EM Validation Summary Report ⓘ

May 16, 2023 – 06:29 PM JST

PDB ID : 7XR3  
EMDB ID : EMD-33404  
Title : 3.4 Angstrom cryoEM D5 reconstruction of mud crab reovirus  
Authors : Zhang, Q.F.; Gao, Y.Z.  
Deposited on : 2022-05-09  
Resolution : 3.70 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](mailto: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>.

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

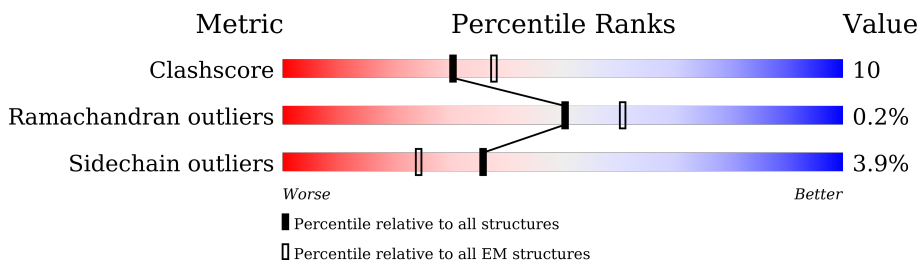
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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.



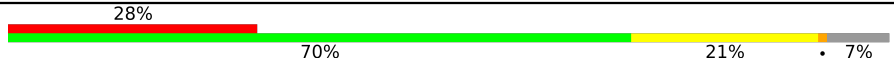


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	854	
1	B	854	
1	C	854	
1	D	854	
1	E	854	
1	F	854	
1	G	854	
1	H	854	

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Mol	Chain	Length	Quality of chain
1	I	854	
1	J	854	
2	Z	1425	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 76250 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 VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	815	Total 6516	C 4128	N 1128	O 1232	S 28	0	0
1	B	846	Total 6746	C 4260	N 1175	O 1283	S 28	0	0
1	C	794	Total 6372	C 4043	N 1100	O 1201	S 28	0	0
1	D	846	Total 6746	C 4260	N 1175	O 1283	S 28	0	0
1	E	794	Total 6372	C 4043	N 1100	O 1201	S 28	0	0
1	F	846	Total 6746	C 4260	N 1175	O 1283	S 28	0	0
1	G	794	Total 6372	C 4043	N 1100	O 1201	S 28	0	0
1	H	846	Total 6746	C 4260	N 1175	O 1283	S 28	0	0
1	I	794	Total 6372	C 4043	N 1100	O 1201	S 28	0	0
1	J	846	Total 6746	C 4260	N 1175	O 1283	S 28	0	0

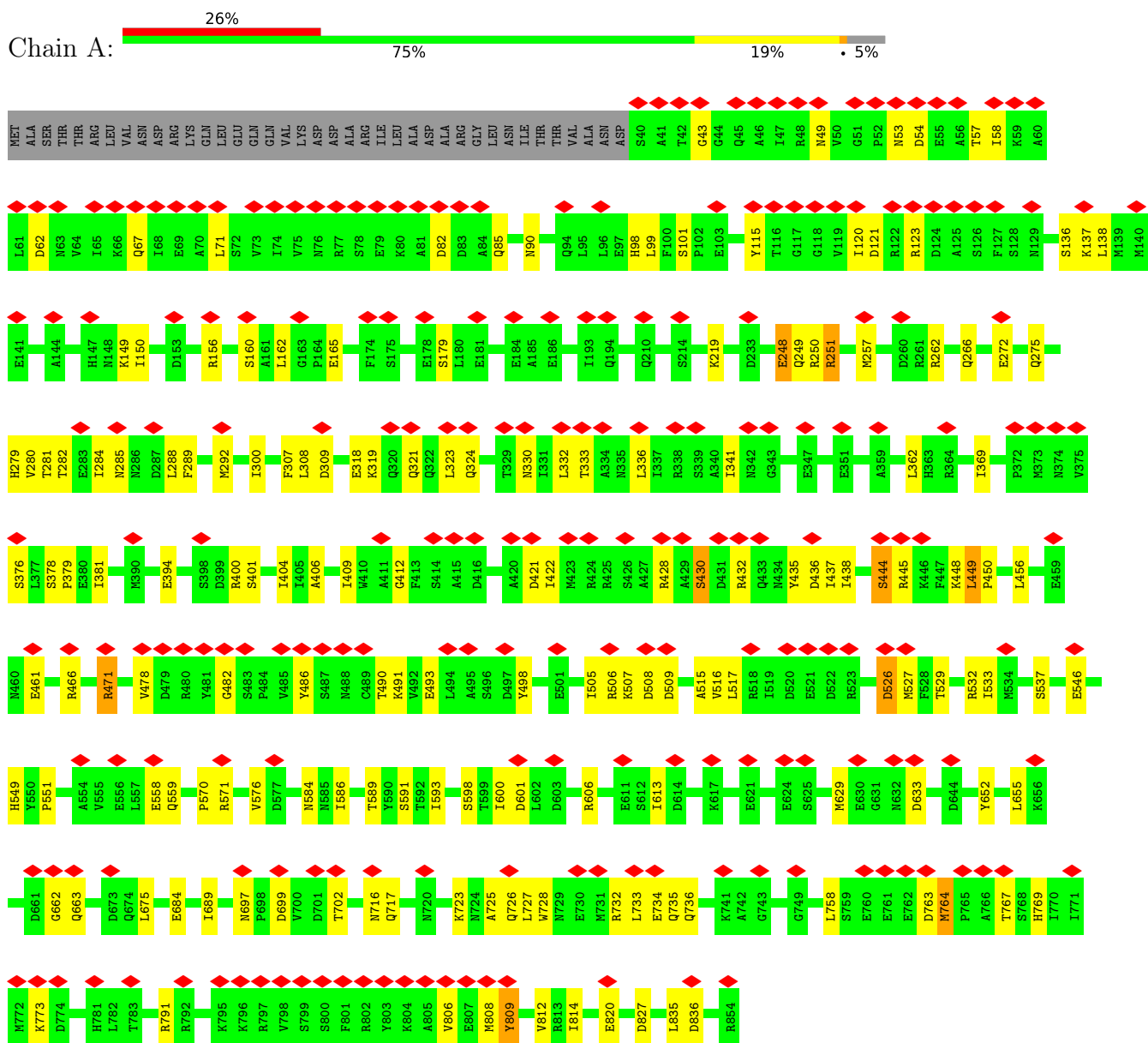
- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Z	1320	Total 10516	C 6661	N 1799	O 2000	S 56	0	0

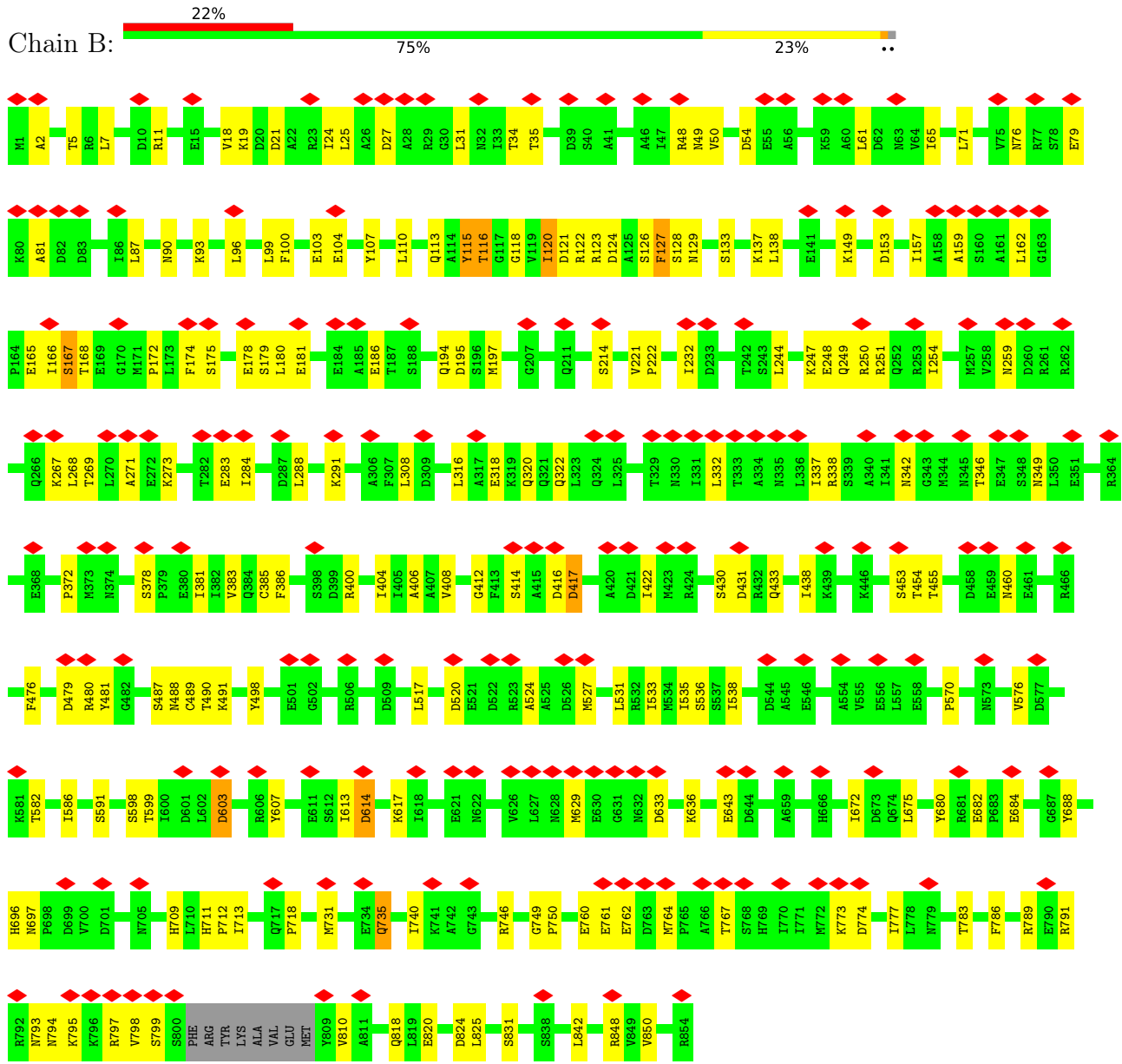
### 3 Residue-property plots [i](#)

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.

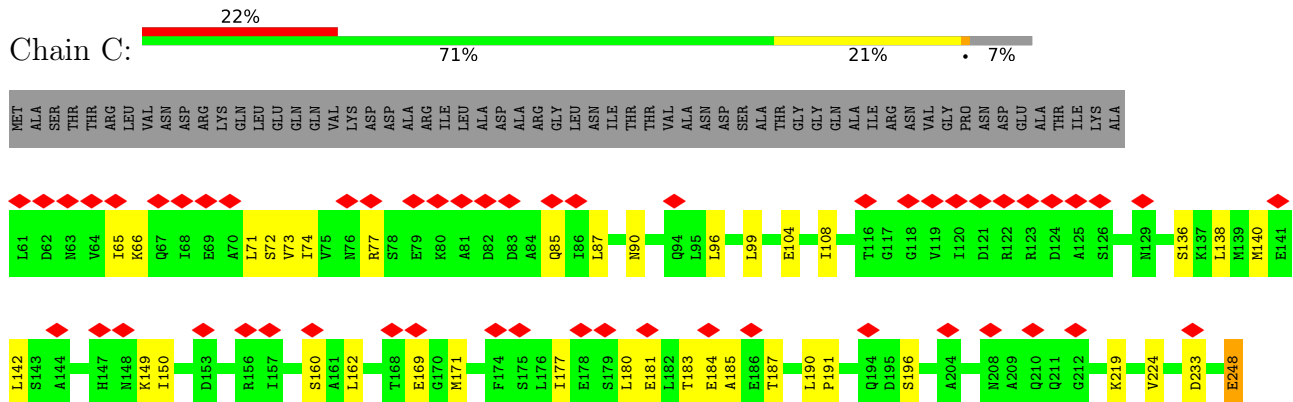
- Molecule 1: VP3

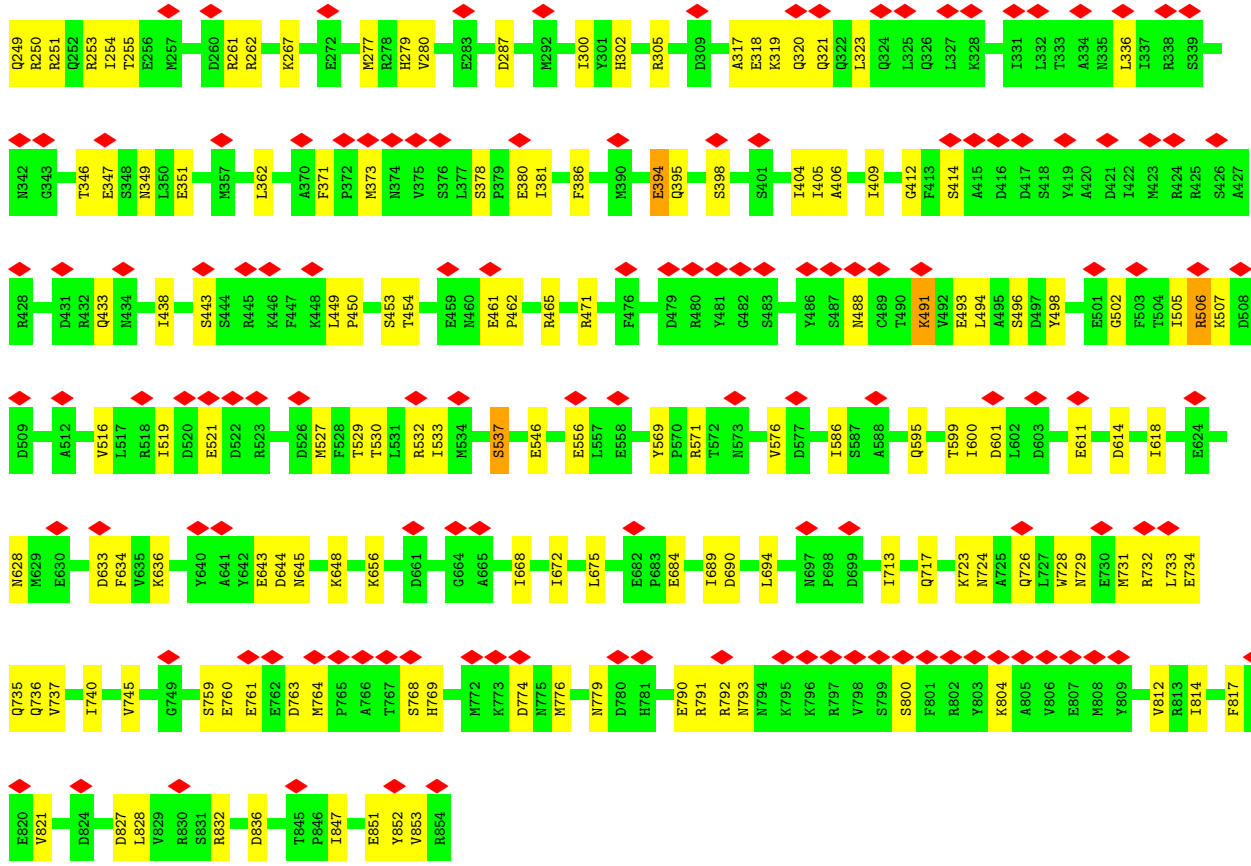


- Molecule 1: VP3

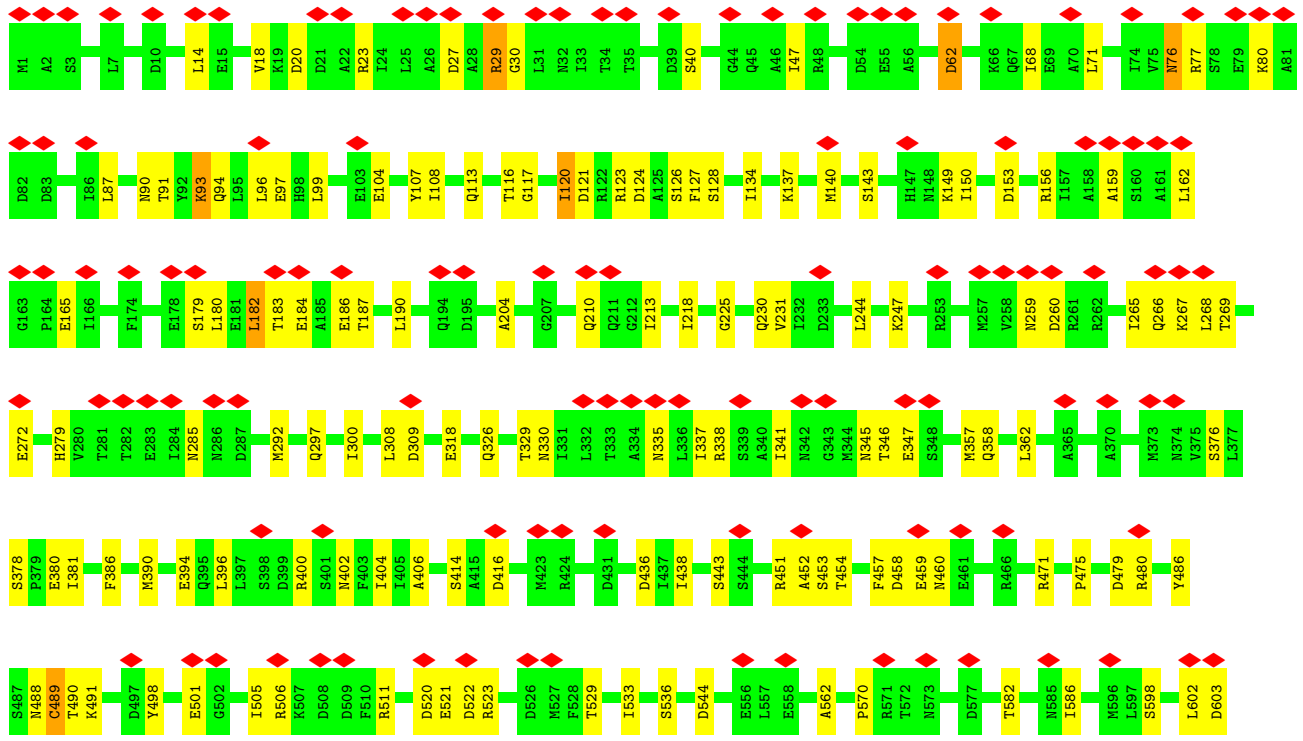
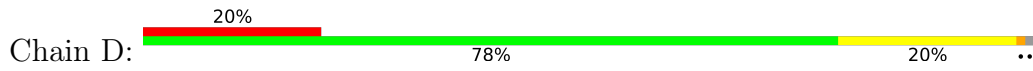


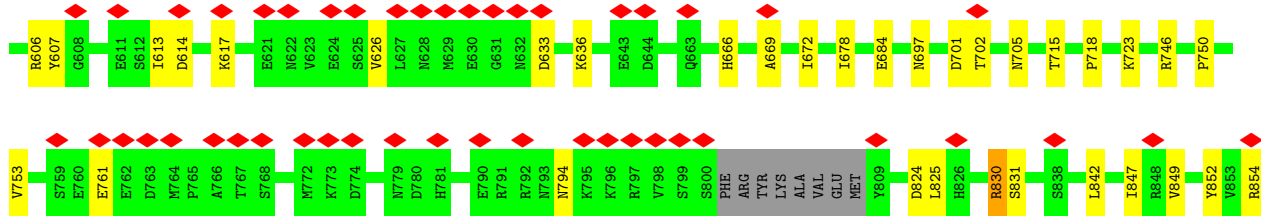
• Molecule 1: VP3



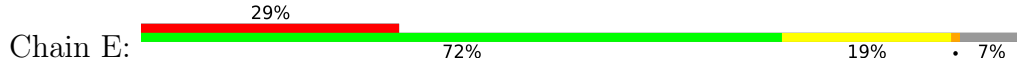


• Molecule 1: VP3

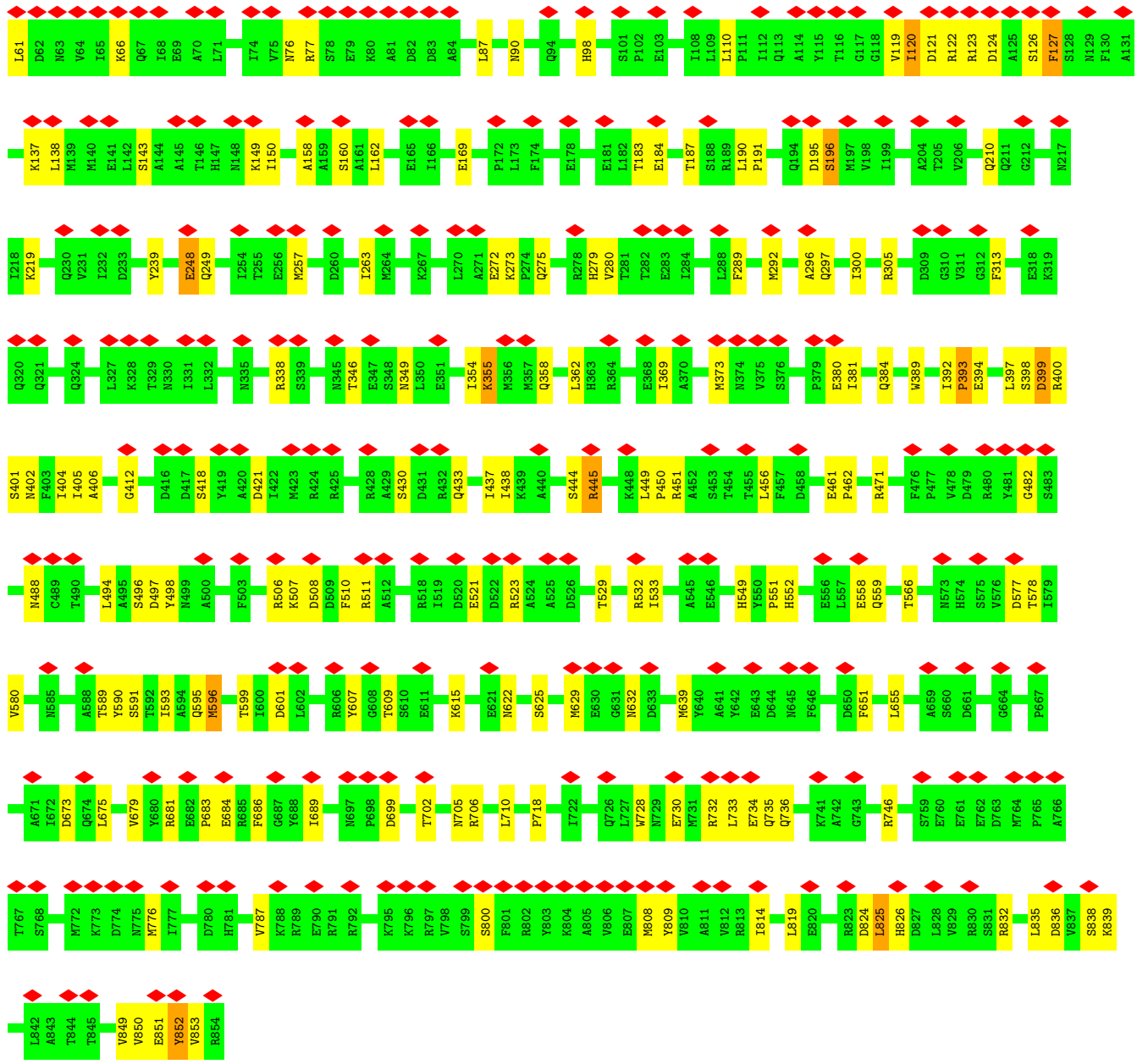




• Molecule 1: VP3

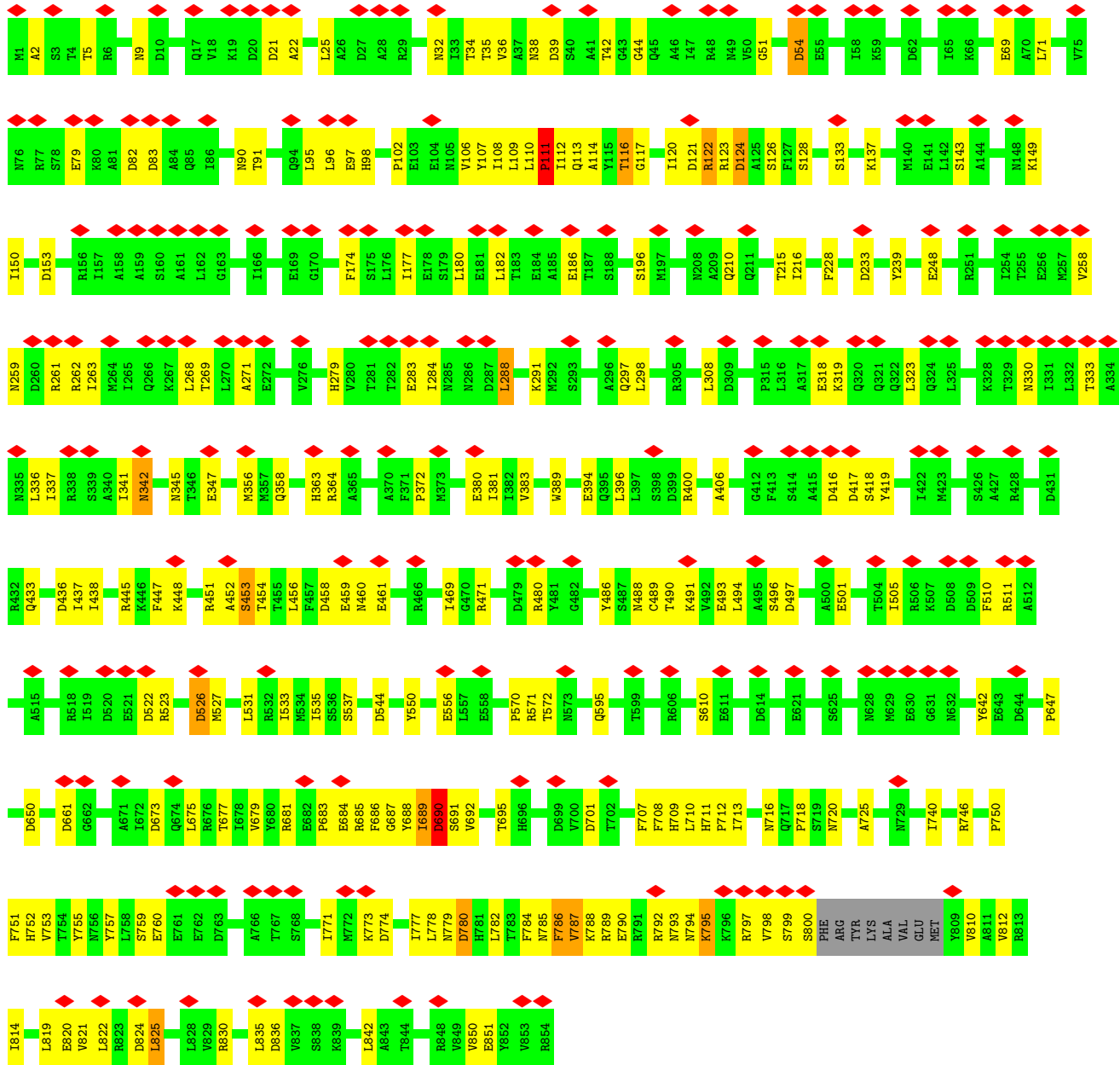


MET	ALA	SER	THR	THR	ARG	LEU	VAL	ASN	ASP	ARG	LYS	GLN	LEU	GLU	GLN	GLN	VAL	VAL	LYS	ASP	ASP	ALA	ARG	ILE	LEU	ALA	ASP	ALA	ARG	GLY	LEU	ASN	LEU	ASN	ILE	THR	THR	THR	VAL	ALA	ASN	ASP	ALA	ARG	ALA	LYS	THR	GLY	GLY	GLN	ALA	ILE	ARG	ASN	VAL	PRO	GLY	ASN	ASP	ASP	GLU	ALA	ALA	THR	ILE	LYS	ALA
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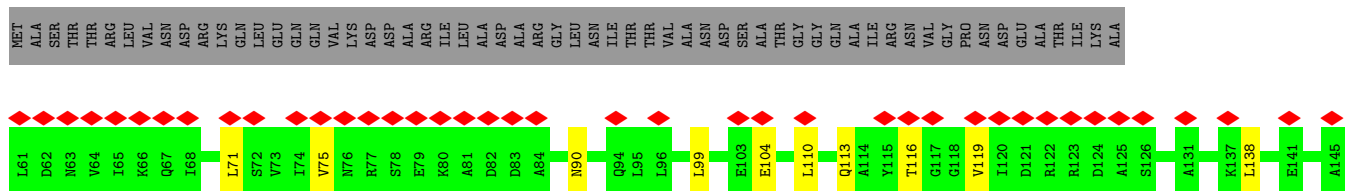
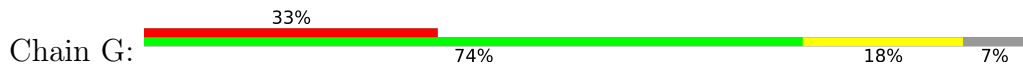


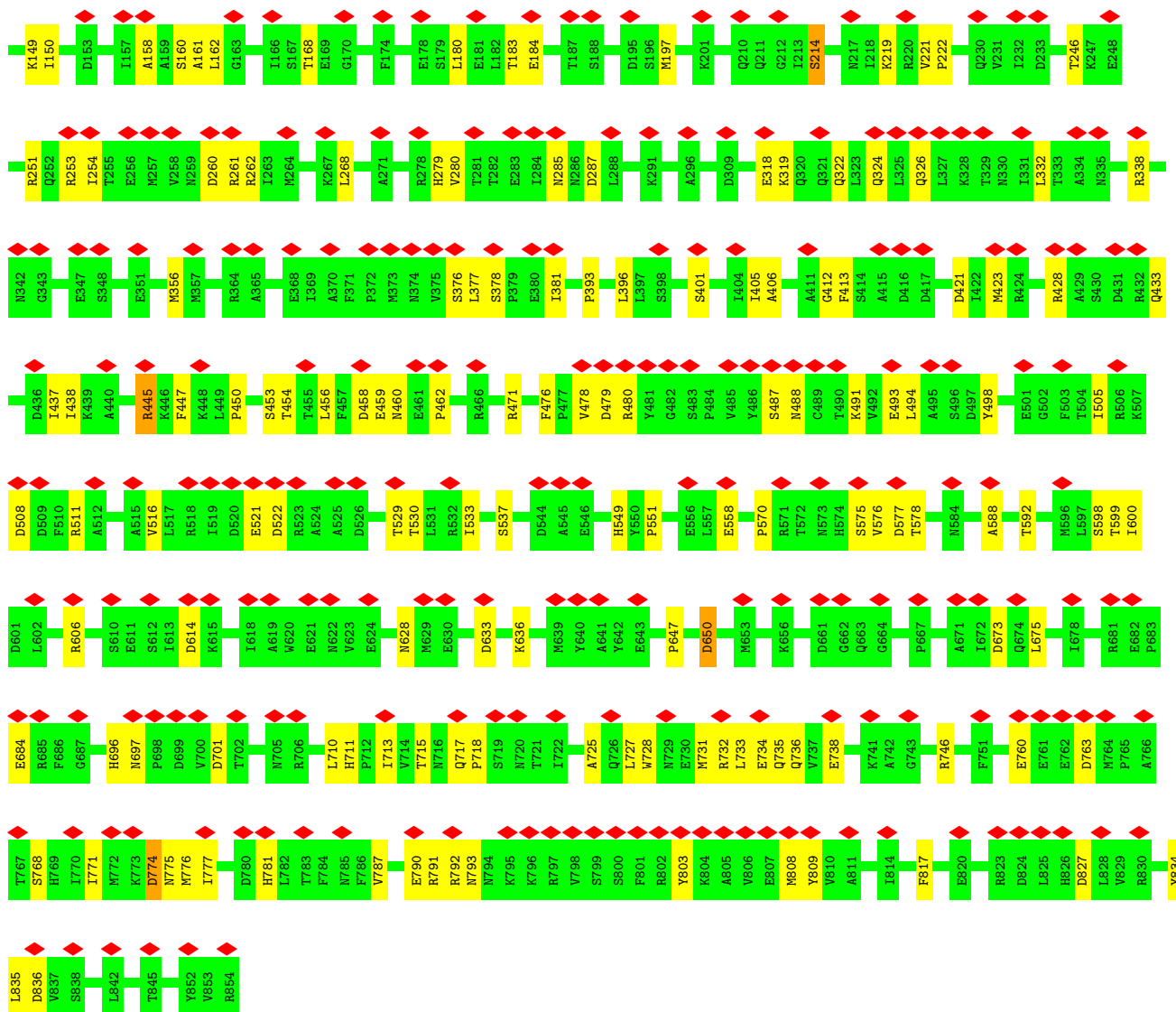


• Molecule 1: VP3

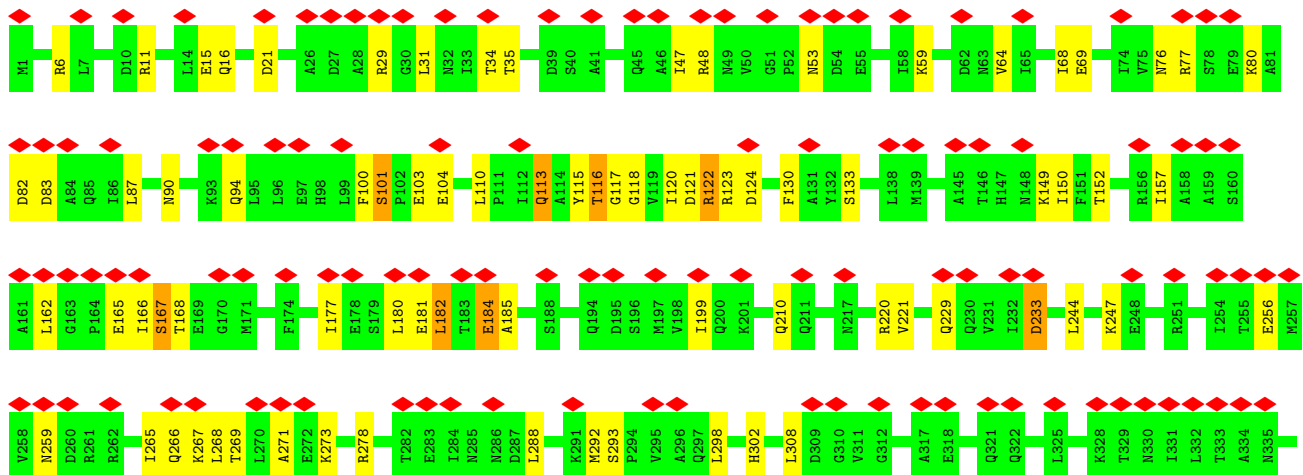
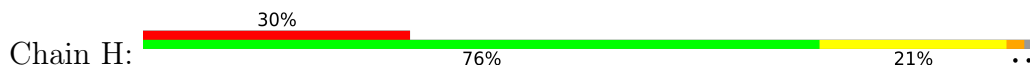


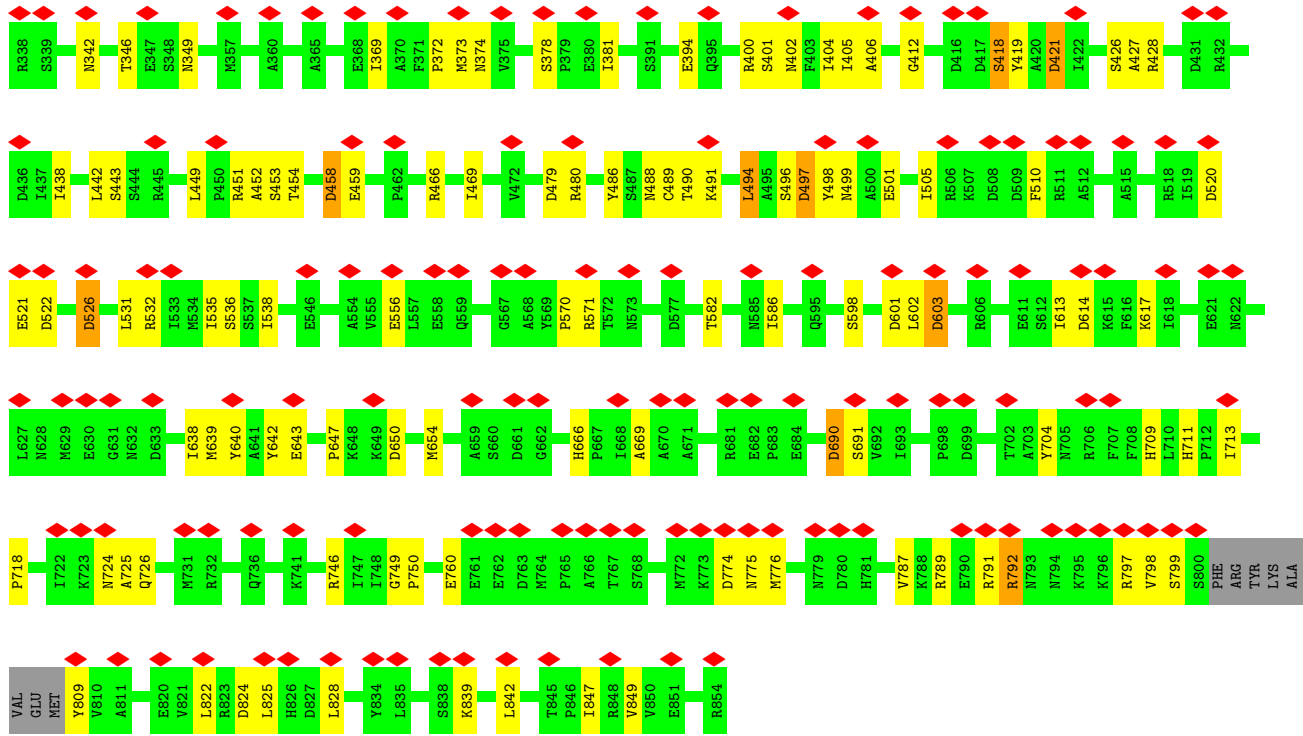
• Molecule 1: VP3



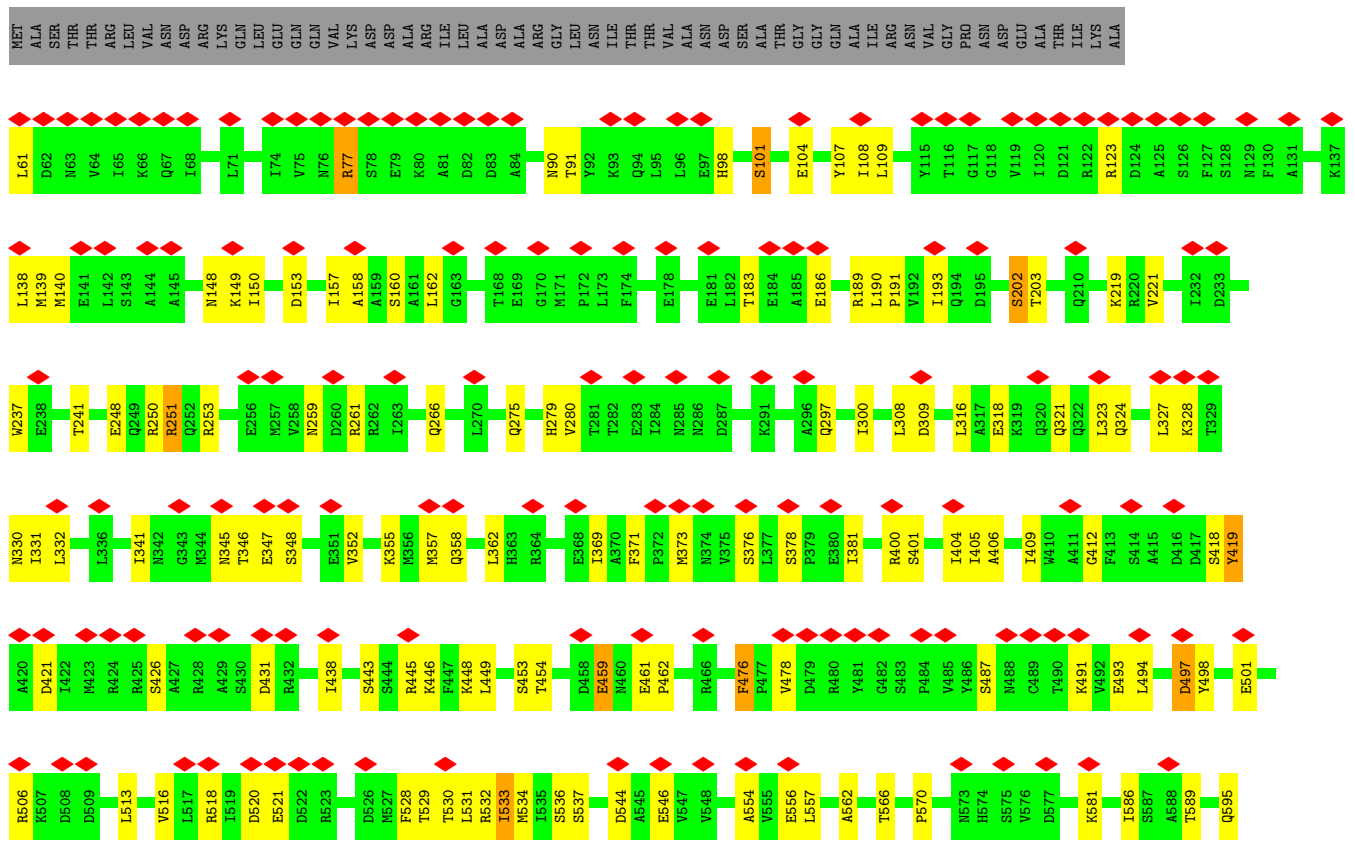


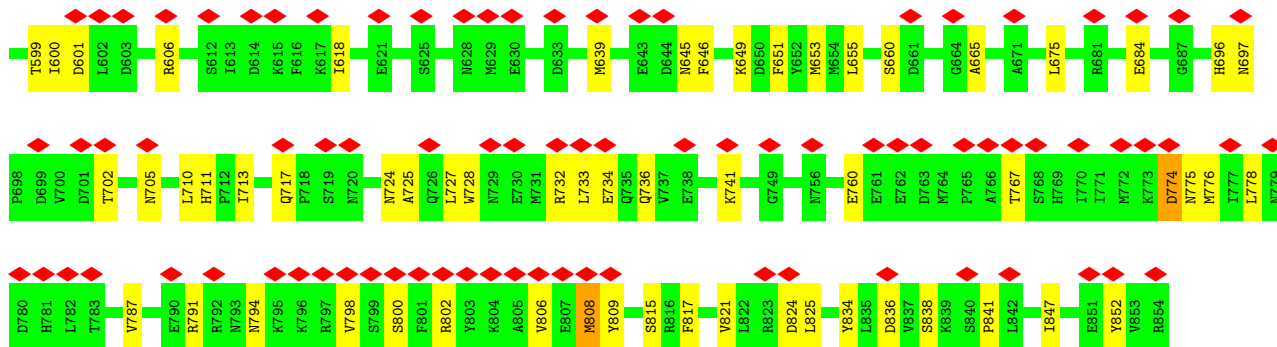
• Molecule 1: VP3



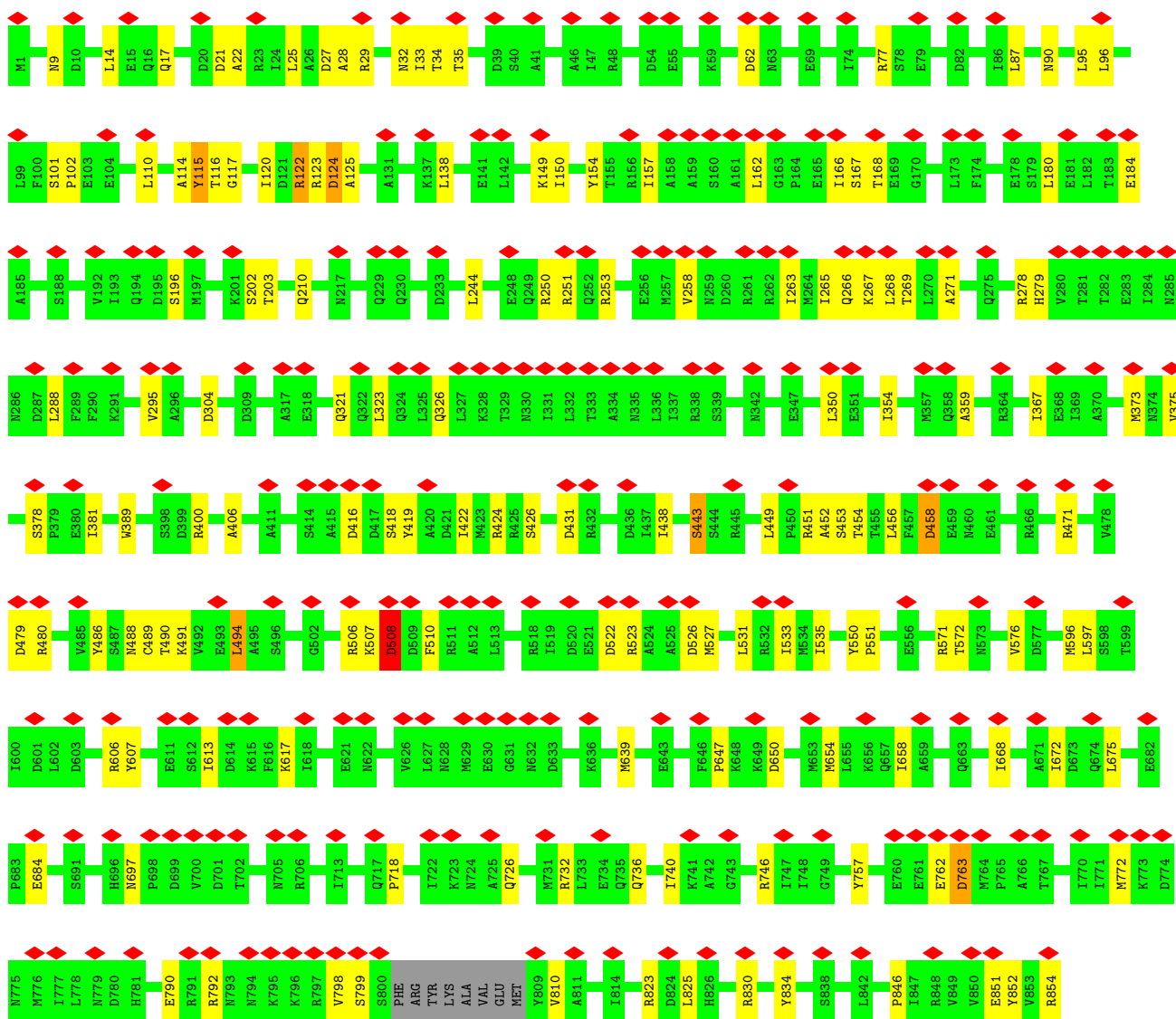
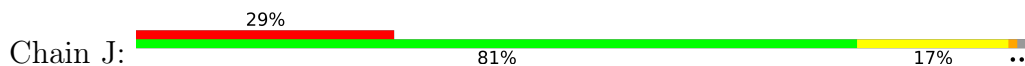


• Molecule 1: VP3





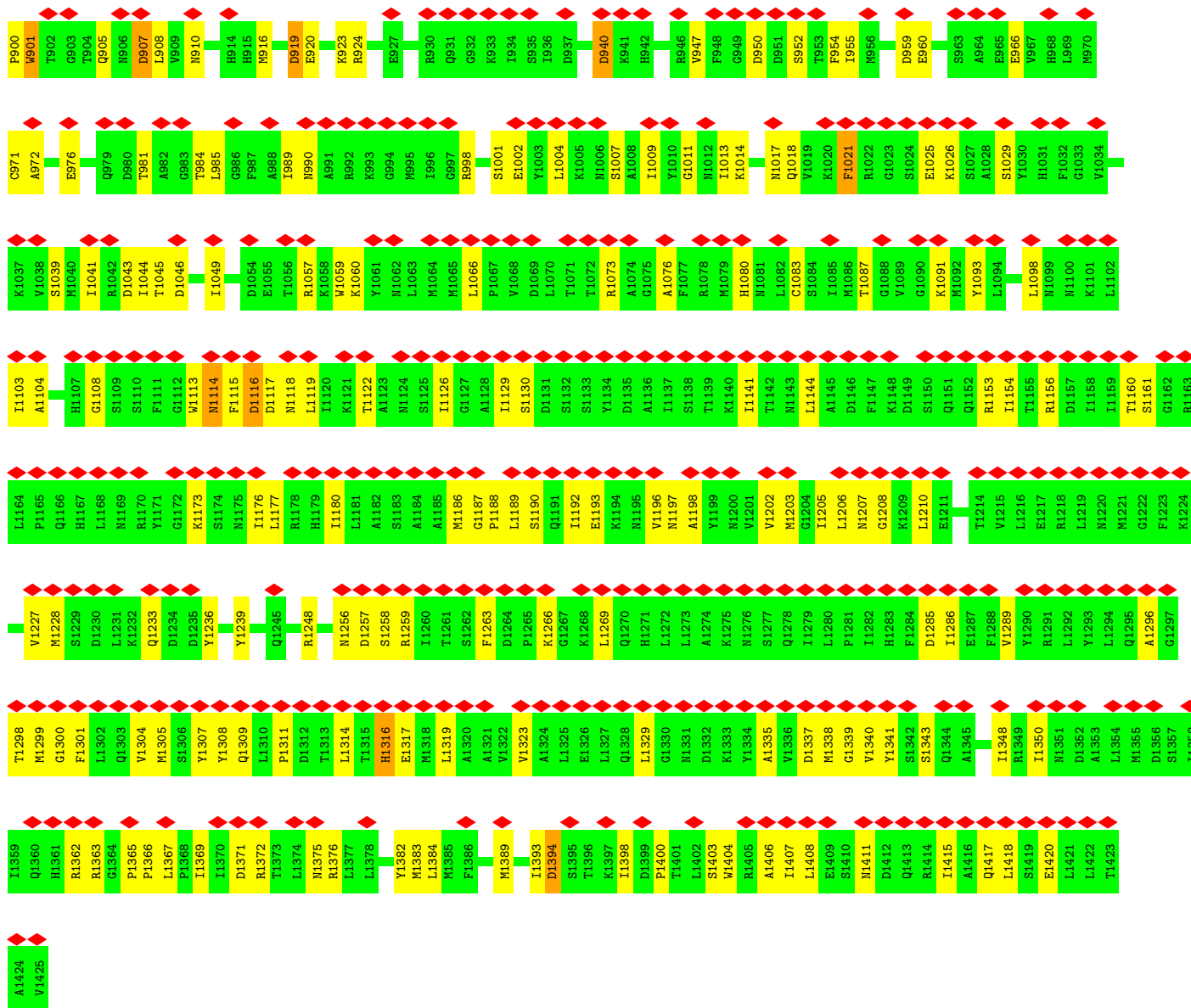
• Molecule 1: VP3



• Molecule 2: VP1



MET	ARG	ILE	MET	ALA	GLN	ARG	LEU	LYS	LEU	GLU	GLN	ARG	GLU	ILE	ASP	LYS	LYS	LYS	LYS	GLU	ILE	ASP	LYS	V52	S53	P54	F55	L56	D57	S58	T59	P60																										
R61	T62	T63	L64	H65	H66	S67	G70	Q71	Q72	L73	H74	S75	L76	D77	D78	E79	L80	A81	Q82	L83	C84	L206	L85	L86	E87	E88	E89	L90	Q91	L92	Q93	D96	E97	Q98	L99	T100	A101	L102	L103	L104	F105	L106	T107	T110	G111	S112	P113	Q114	E115	I116	Q117	V119	D120	K121	E122	W123		
M124	K125	S126	H129	V130	P131	S132	F133	L134	G135	D136	V137	K138	L139	M140	F141	GLY	ASP	THR	ALA	GLY	LYS	PHE	ARG	SER	SER	THR	SER	LYS	VAL	ASP	ASP	ILE	HIS	SER	ILE	THR	THR	SER	ASP	VAL	GLN	VAL	THR	THR	GLN	THR	ARG	SER	GLN	ILE	ARG	ASP	ASN	S190	Y181	R182	V183	Q184
K185	K186	H187	K188	V189	Q190	P192	L193	K194	P195	H196	T197	D200	Y201	K202	Y203	K204	G205	L206	P207	R208	V209	V210	L211	R212	F213	V214	P215	K216	V217	D218	T219	T220	S221	ASN	SER	ASN	ASN	ARG	LYS	ASP	LYS	SER	SER	ALA	ALA	F236	S239	C240	D241	D242	L243	S244						
P245	T246	W247	K248	Y249	T252	E253	A254	K255	E256	A257	F258	P259	D260	R261	Y262	S263	S264	D265	C266	L267	H268	P269	M270	T271	W272	E273	E274	W275	L276	E277	E278	W279	Q280	L286	T287	Q288	Y289	A290	H291	Q292	L293	V296	T297	L298	L299	Q300	D301	F302	N303	L304	G309	A310	S311	R312	V313			
R314	N315	I316	D317	M318	S319	T320	L321	P322	T323	S324	I325	N326	V327	L328	D329	H330	F331	E332	L333	Y334	G335	L336	D337	A337	M339	K340	E341	Y342	V343	R344	S345	G346	E347	W348	Y349	G350	L351	L352	R353	E354	I355	E356	Q357	E358	G359	M360	T361	V362	N363	S365	E366	K367	V368	F369	A370	N371	P372	D373
T374	Y375	V376	L377	M378	V379	K380	K381	L384	R385	R386	F387	Q388	Q389	E390	I391	A392	S393	M396	T397	P398	K402	L403	T400	E401	A402	L403	M405	L406	M407	F408	Y409	H410	W411	M412	V415	T416	A417	E418	P419	Q422	W423	I424	K425	D426	D427	L428	L429	K430	S433	R434	Y435	D438	A439					
T440	F441	D442	Y443	M444	K446	R447	S448	E449	M450	T451	V452	W453	T454	R455	Y456	H457	L458	A459	A460	H461	K462	V463	L464	E465	C466	A467	L468	R469	I470	V471	E472	Y475	L476	D478	I479	Q480	D481	E482	T483	F484	K485	D486	I487	L488	I489	D490	L491	G492	L494	I495	M496	R497	D498	P499	I500			
Y501	G502	T503	T504	R507	D508	A509	T510	V511	M513	K514	Q515	L516	M517	Y518	T519	Q520	G521	T522	Q523	F524	R525	R526	L527	M528	F529	K530	D533	Y534	S535	N536	F537	A538	E539	K540	L543	K544	G545	E546	Q547	M548	T549	N550	E551	P552	P553	T554	L555	L556	A557	T558	T559	H560	Y561	E562	E563			
M564	D565	K566	K567	R568	I569	D570	A571	L572	I573	N576	Q577	R578	A579	G580	N581	I582	L583	S584	Q585	S586	S587	I588	E589	R590	C591	R592	Y593	T594	D595	S596	L597	D598	L599	V600	G601	D602	N604	R605	Y606	F607	S608	L613	G618	F619	A620	S621	S622	D623	L624	L625	S626	G627	I629	D630				
S631	N632	E633	S634	I635	E636	F637	T638	A641	H642	L643	R644	K645	E653	Q654	I655	S661	T662	V663	P664	R665	P666	S667	L668	P669	M670	V671	L672	L673	S674	D595	S596	L597	D598	L599	G601	D602	N604	R605	Y606	F607	S608	L613	G618	F619	A620	S621	S622	D623	L624	L625	S626	G627	I629	D630				
S702	L703	M704	L705	V706	E707	S708	T709	V710	E711	M712	S713	T714	R715	Q716	K717	L718	M720	L721	P664	R665	P666	S667	L668	M670	V671	L672	L673	S674	D595	S596	L597	D598	L599	G601	D602	N604	R605	Y606	F607	S608	L613	G618	F619	A620	S621	S622	D623	L624	L625	S626	G627	I629	D630					
P762	Y763	H764	L765	A766	G767	L769	L770	F771	D775	L776	M779	A780	M781	K782	K783	Y784	R785	G786	V787	S788	M789	K790	Y791	G792	Q793	G794	I795	S796	M797	A798	T799	P800	H801	L802	G803	V804	P805	E806	L807	V810	D813	T817	C818	L819	A820	L821	D822	V823	S824	A825	F826	D827						
K831	Y832	T833	E834	A835	D836	L837	E838	M841	R842	D843	G844	S848	E849	I850	G855	E856	T857	V858	L859	E860	R861	M862	N863	F864	A865	D866	L867	N870	N874	T875	P876	P877	R878	L802	G803	V804	P805	E806	L807	V810	D813	T817	C818	L819	A820	L821	D822	V823	S824	A825	F826	D827						



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	128440	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	33.537	Depositor
Minimum map value	-21.310	Depositor
Average map value	0.081	Depositor
Map value standard deviation	1.814	Depositor
Recommended contour level	6.0	Depositor
Map size ( $\text{\AA}$ )	872.0, 872.0, 872.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.09, 1.09, 1.09	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	A	0.32	0/6644	0.55	1/9015 (0.0%)
1	B	0.32	0/6871	0.56	1/9322 (0.0%)
1	C	0.31	0/6499	0.54	1/8818 (0.0%)
1	D	0.34	0/6871	0.55	0/9322
1	E	0.32	0/6499	0.56	2/8818 (0.0%)
1	F	0.34	0/6871	0.57	2/9322 (0.0%)
1	G	0.30	0/6499	0.53	1/8818 (0.0%)
1	H	0.32	0/6871	0.56	1/9322 (0.0%)
1	I	0.32	0/6499	0.55	1/8818 (0.0%)
1	J	0.32	0/6871	0.56	3/9322 (0.0%)
2	Z	0.40	0/10724	0.59	1/14518 (0.0%)
All	All	0.33	0/77719	0.56	14/105415 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	614	ASP	CB-CG-OD1	5.91	123.62	118.30
1	I	774	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	774	ASP	CB-CG-OD1	5.40	123.16	118.30
1	E	699	ASP	CB-CG-OD1	5.35	123.12	118.30
1	E	673	ASP	CB-CG-OD1	5.28	123.06	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6516	0	6517	104	0
1	B	6746	0	6755	144	0
1	C	6372	0	6375	117	0
1	D	6746	0	6755	118	0
1	E	6372	0	6375	124	0
1	F	6746	0	6755	180	0
1	G	6372	0	6375	115	0
1	H	6746	0	6755	138	0
1	I	6372	0	6375	130	0
1	J	6746	0	6755	107	0
2	Z	10516	0	10497	329	0
All	All	76250	0	76289	1515	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 10.

The worst 5 of 1515 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:Z:895:ASN:HB3	2:Z:905:GLN:OE1	1.66	0.96
1:F:98:HIS:HB2	1:F:112:ILE:HD11	1.44	0.96
2:Z:686:PRO:HG3	2:Z:717:LYS:HA	1.48	0.94
1:B:126:SER:HB3	1:B:129:ASN:OD1	1.68	0.93
1:E:119:VAL:HB	1:F:69:GLU:OE2	1.68	0.92

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	813/854 (95%)	741 (91%)	72 (9%)	0	<b>100</b>   <b>100</b>
1	B	842/854 (99%)	775 (92%)	65 (8%)	2 (0%)	47   78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	792/854 (93%)	721 (91%)	71 (9%)	0	100	100
1	D	842/854 (99%)	785 (93%)	56 (7%)	1 (0%)	51	83
1	E	792/854 (93%)	719 (91%)	70 (9%)	3 (0%)	34	69
1	F	842/854 (99%)	761 (90%)	76 (9%)	5 (1%)	25	62
1	G	792/854 (93%)	726 (92%)	66 (8%)	0	100	100
1	H	842/854 (99%)	786 (93%)	55 (6%)	1 (0%)	51	83
1	I	792/854 (93%)	733 (93%)	58 (7%)	1 (0%)	51	83
1	J	842/854 (99%)	777 (92%)	64 (8%)	1 (0%)	51	83
2	Z	1314/1425 (92%)	1162 (88%)	144 (11%)	8 (1%)	25	62
All	All	9505/9965 (95%)	8686 (91%)	797 (8%)	22 (0%)	50	78

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	127	PHE
1	F	689	ILE
1	J	115	TYR
2	Z	894	ASP
2	Z	901	TRP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	718/751 (96%)	688 (96%)	30 (4%)	30	59
1	B	744/751 (99%)	716 (96%)	28 (4%)	33	61
1	C	704/751 (94%)	679 (96%)	25 (4%)	35	63
1	D	744/751 (99%)	713 (96%)	31 (4%)	30	59
1	E	704/751 (94%)	681 (97%)	23 (3%)	38	64
1	F	744/751 (99%)	708 (95%)	36 (5%)	25	56
1	G	704/751 (94%)	689 (98%)	15 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	744/751 (99%)	705 (95%)	39 (5%)	23	55
1	I	704/751 (94%)	676 (96%)	28 (4%)	31	60
1	J	744/751 (99%)	722 (97%)	22 (3%)	41	66
2	Z	1167/1263 (92%)	1117 (96%)	50 (4%)	29	58
All	All	8421/8773 (96%)	8094 (96%)	327 (4%)	36	60

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	251	ARG
2	Z	384	LEU
1	I	487	SER
1	J	196	SER
2	Z	591	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	736	GLN
2	Z	704	ASN
2	Z	268	HIS
2	Z	410	HIS
2	Z	748	GLN

### 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.

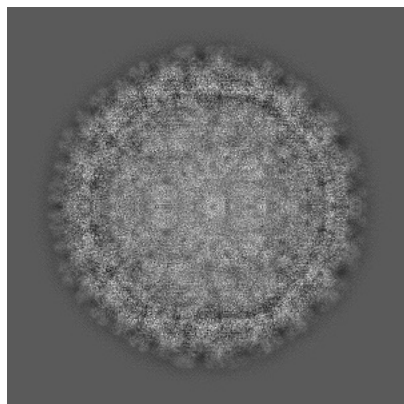
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33404. These allow visual inspection of the internal detail of the map and identification of artifacts.

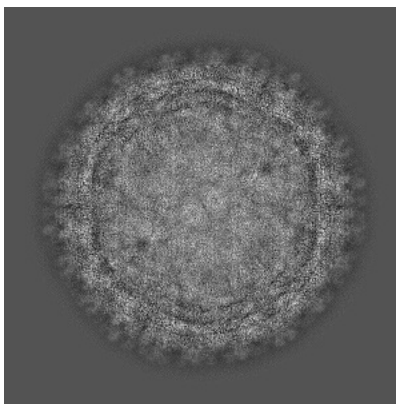
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

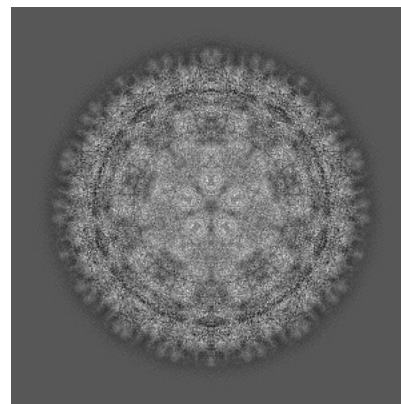
#### 6.1.1 Primary map



X

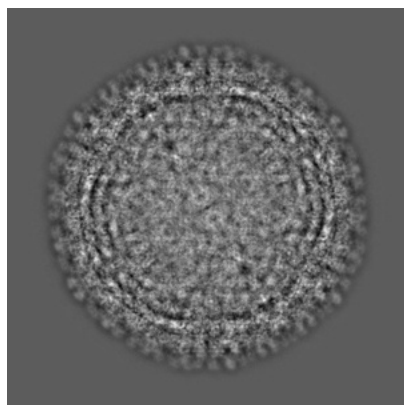


Y

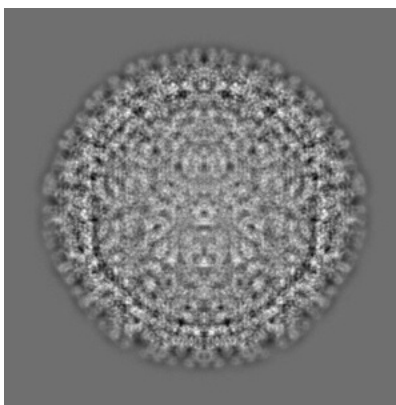


Z

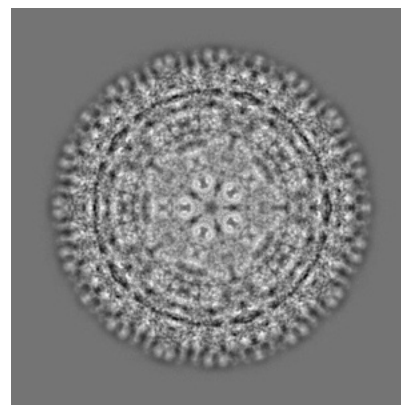
#### 6.1.2 Raw map



X



Y

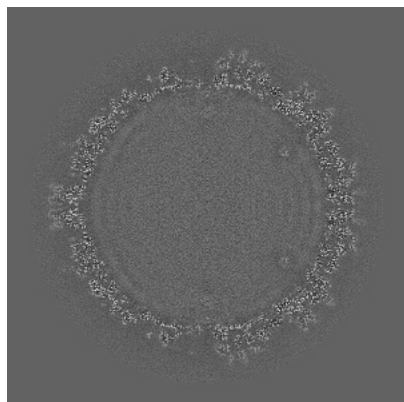


Z

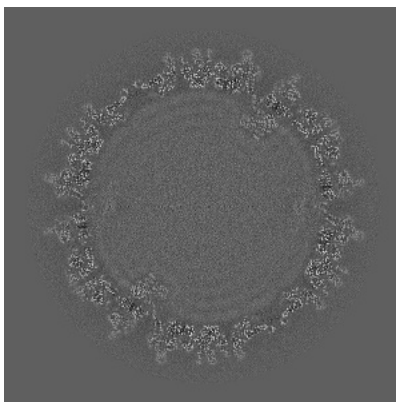
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

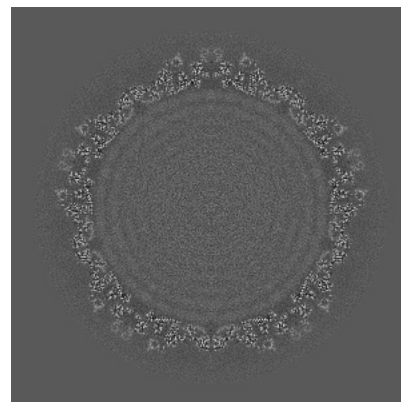
### 6.2.1 Primary map



X Index: 400

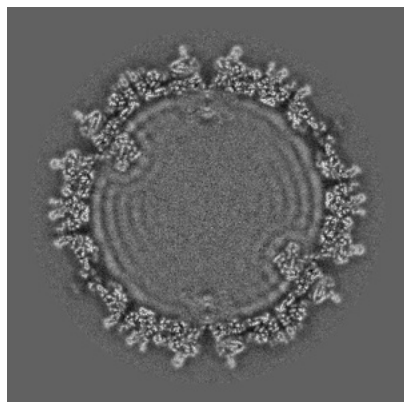


Y Index: 400

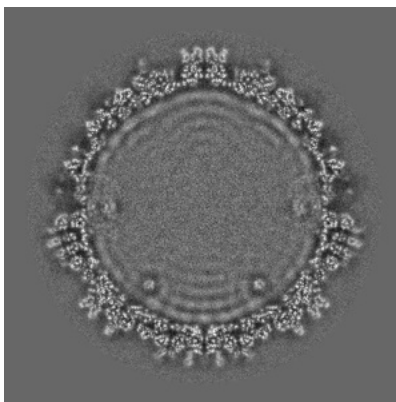


Z Index: 400

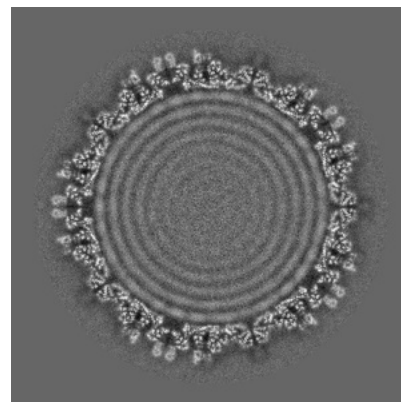
### 6.2.2 Raw map



X Index: 400



Y Index: 400



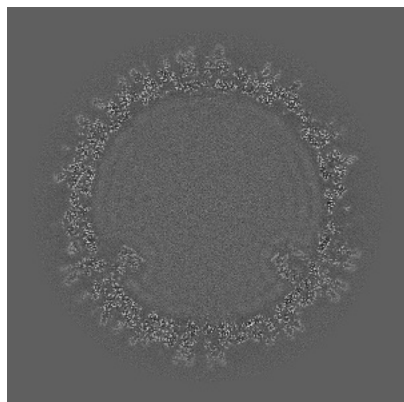
Z Index: 400

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

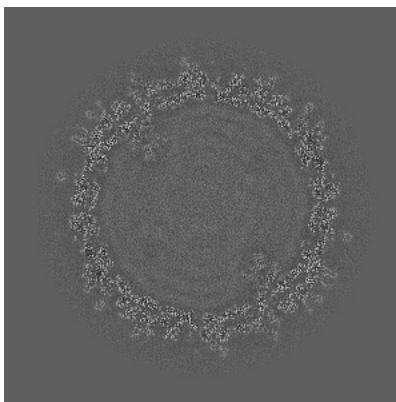


## 6.3 Largest variance slices [i](#)

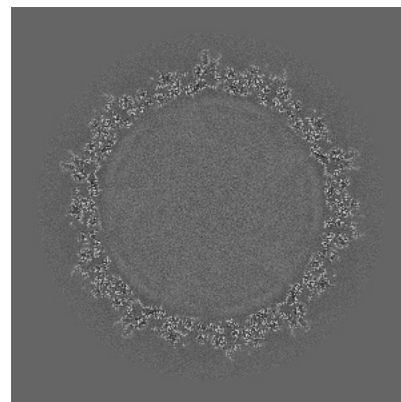
### 6.3.1 Primary map



X Index: 358

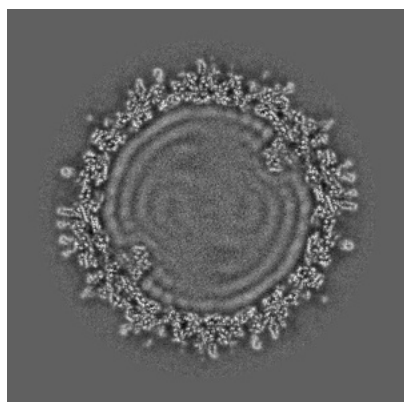


Y Index: 292

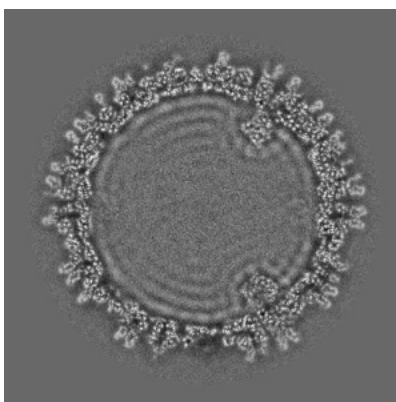


Z Index: 336

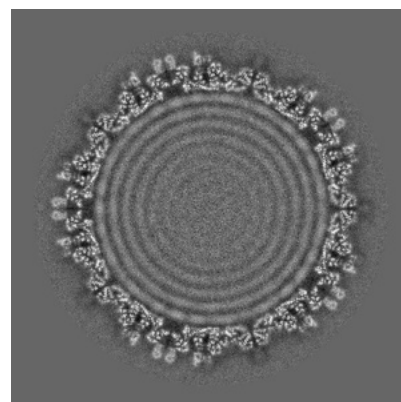
### 6.3.2 Raw map



X Index: 293



Y Index: 354

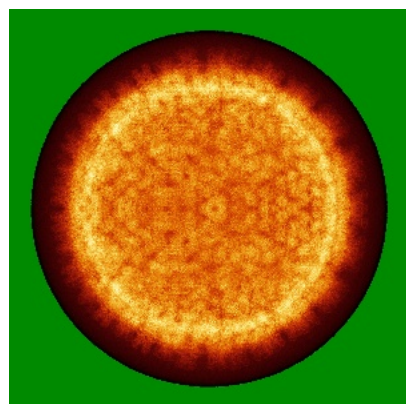


Z Index: 400

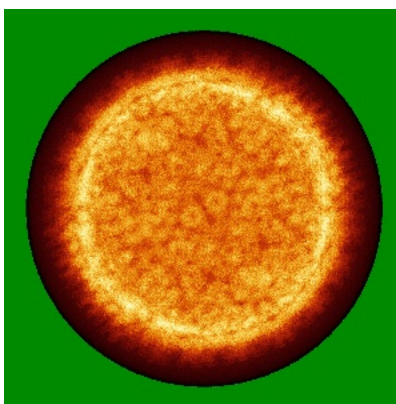
The images above show the largest variance slices of the map in three orthogonal directions.

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

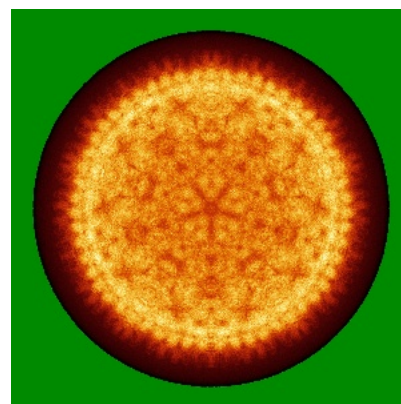
### 6.4.1 Primary map



X

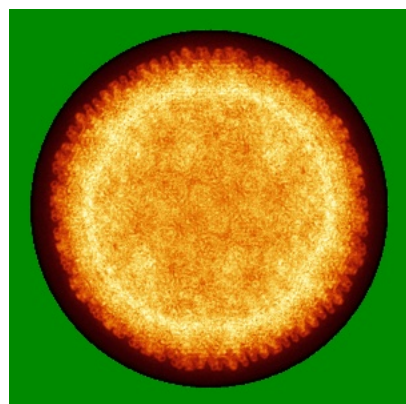


Y

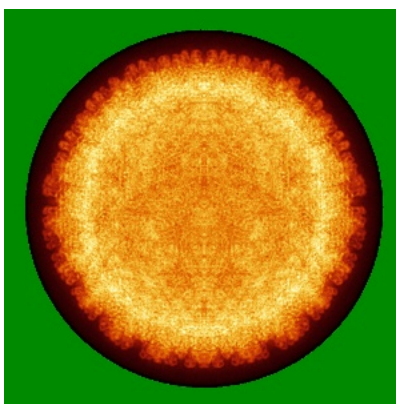


Z

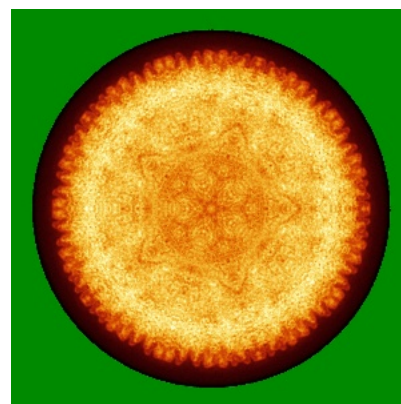
### 6.4.2 Raw map



X



Y



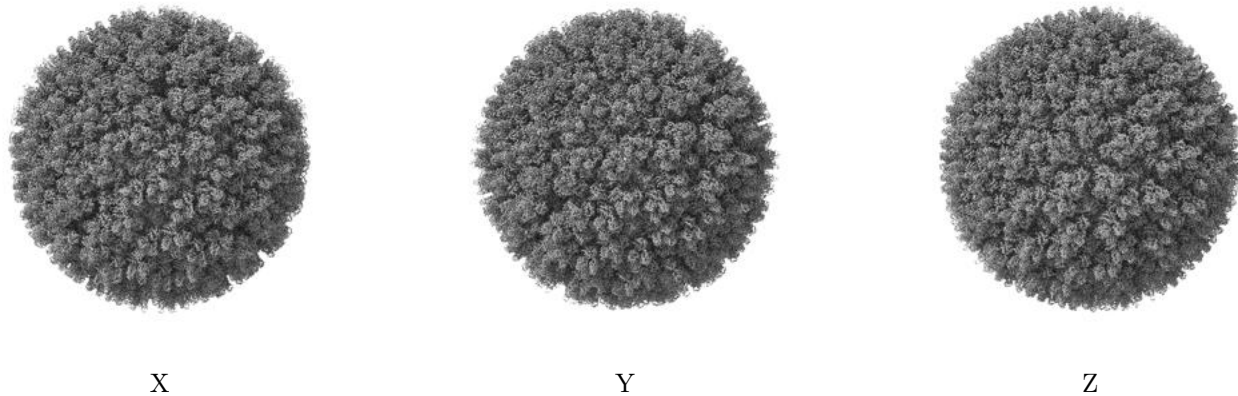
Z

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.



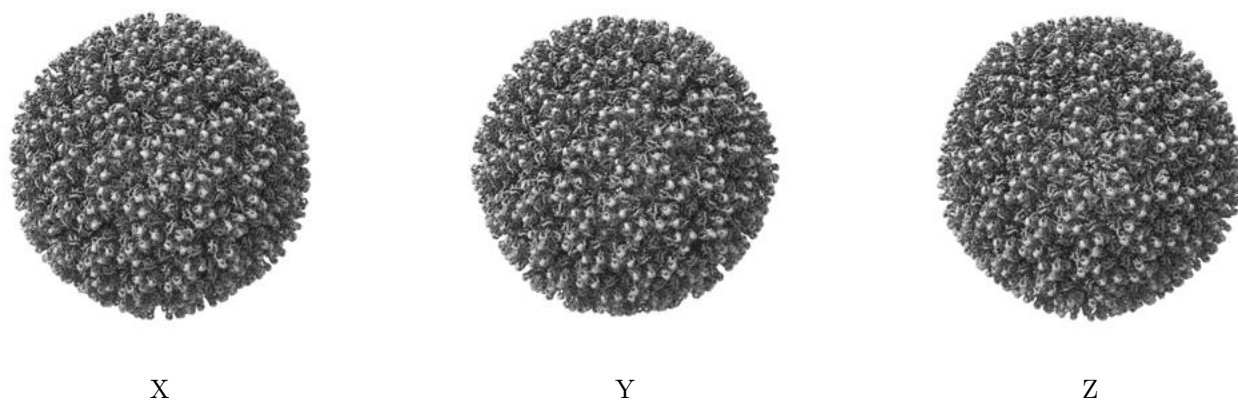
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. 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



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.

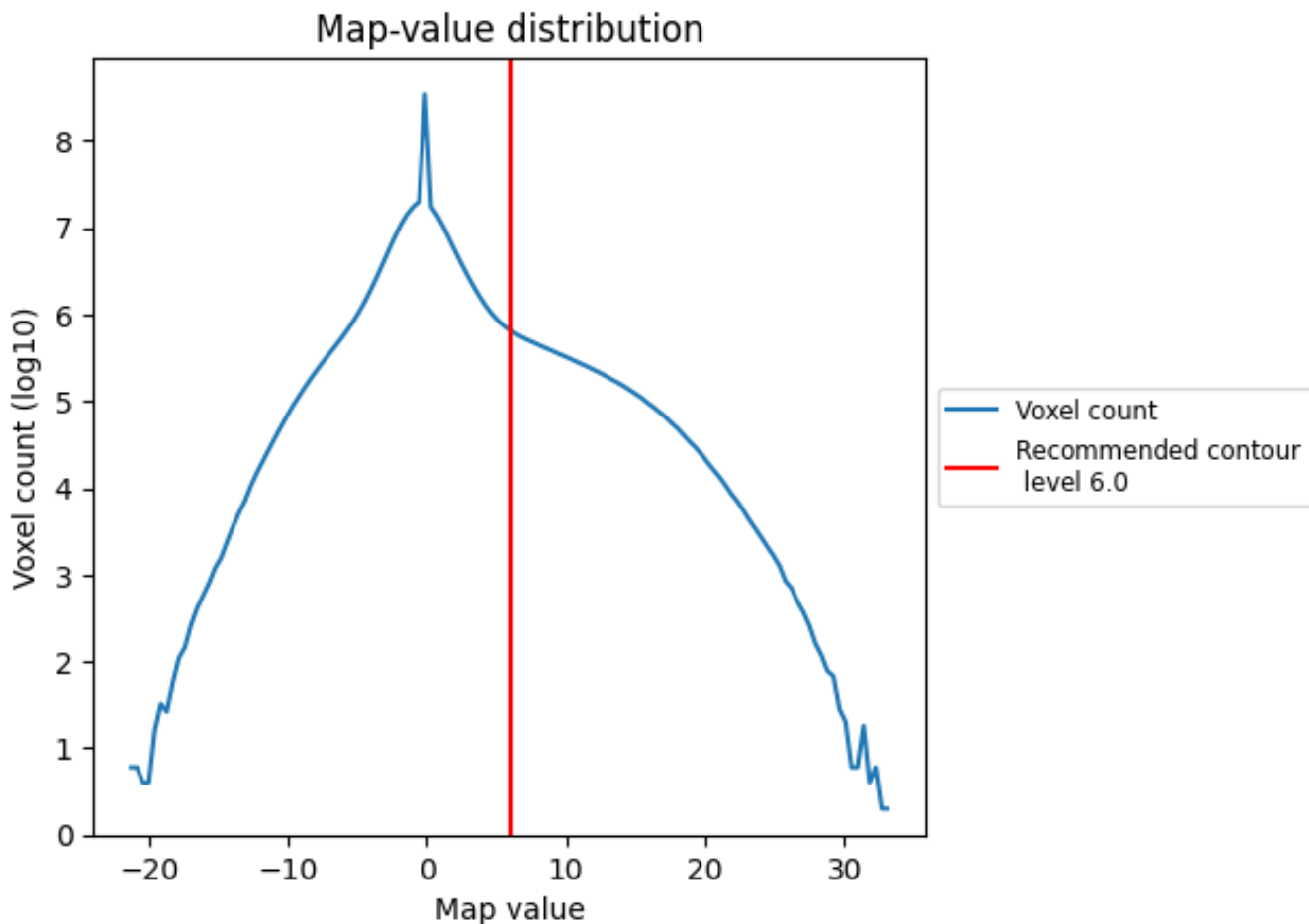
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

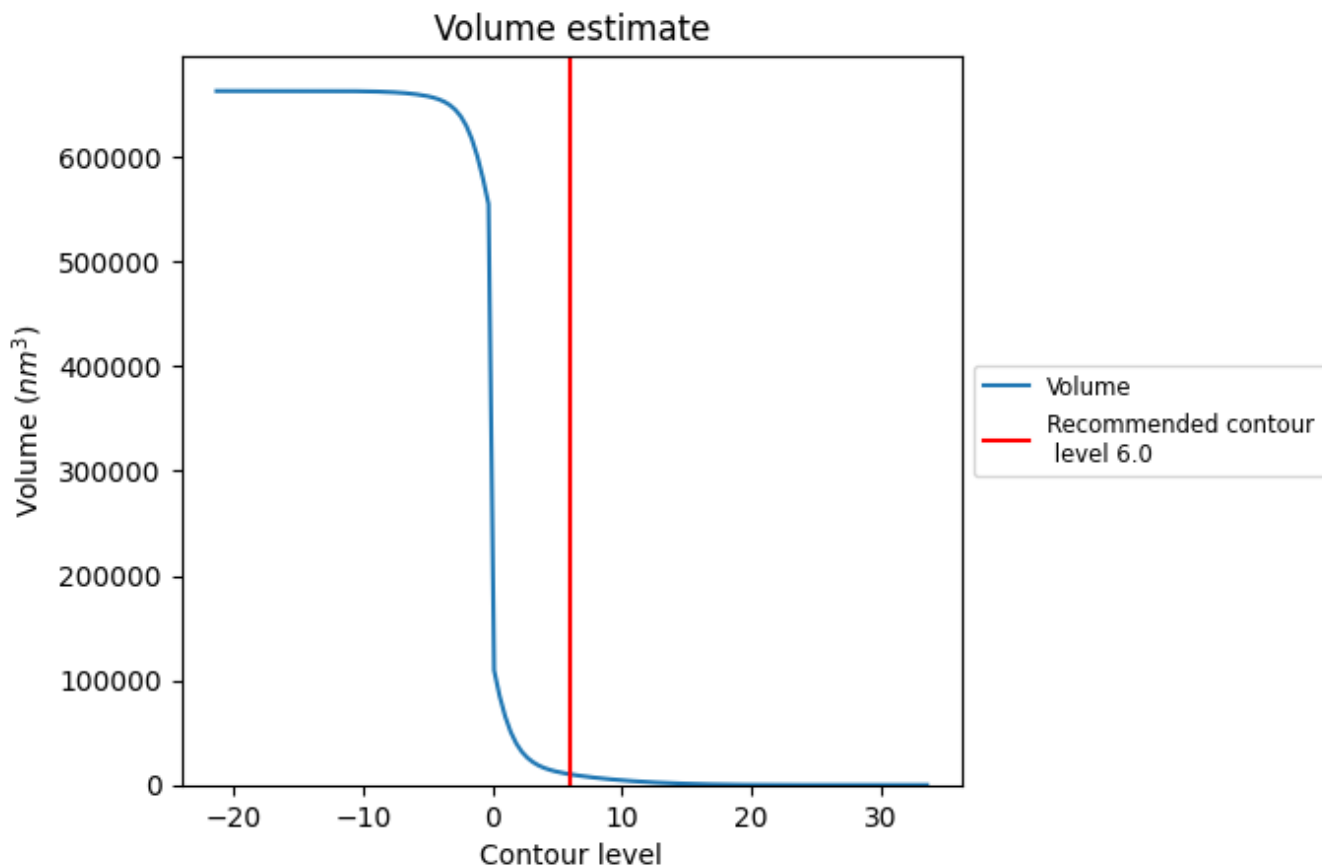
This section contains the results of statistical analysis of the map.

### 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.

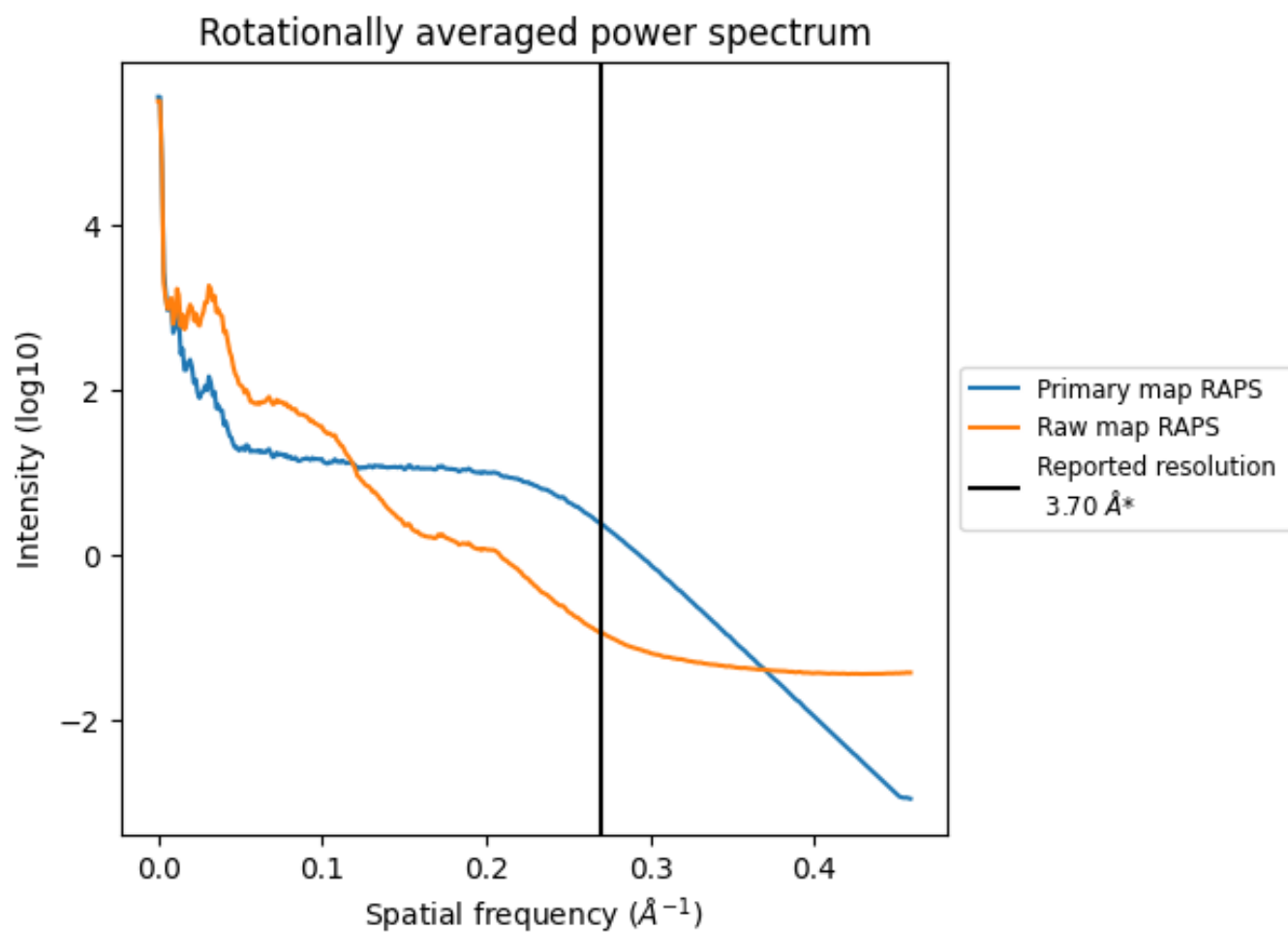
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10162  $\text{nm}^3$ ; this corresponds to an approximate mass of 9180 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](#)

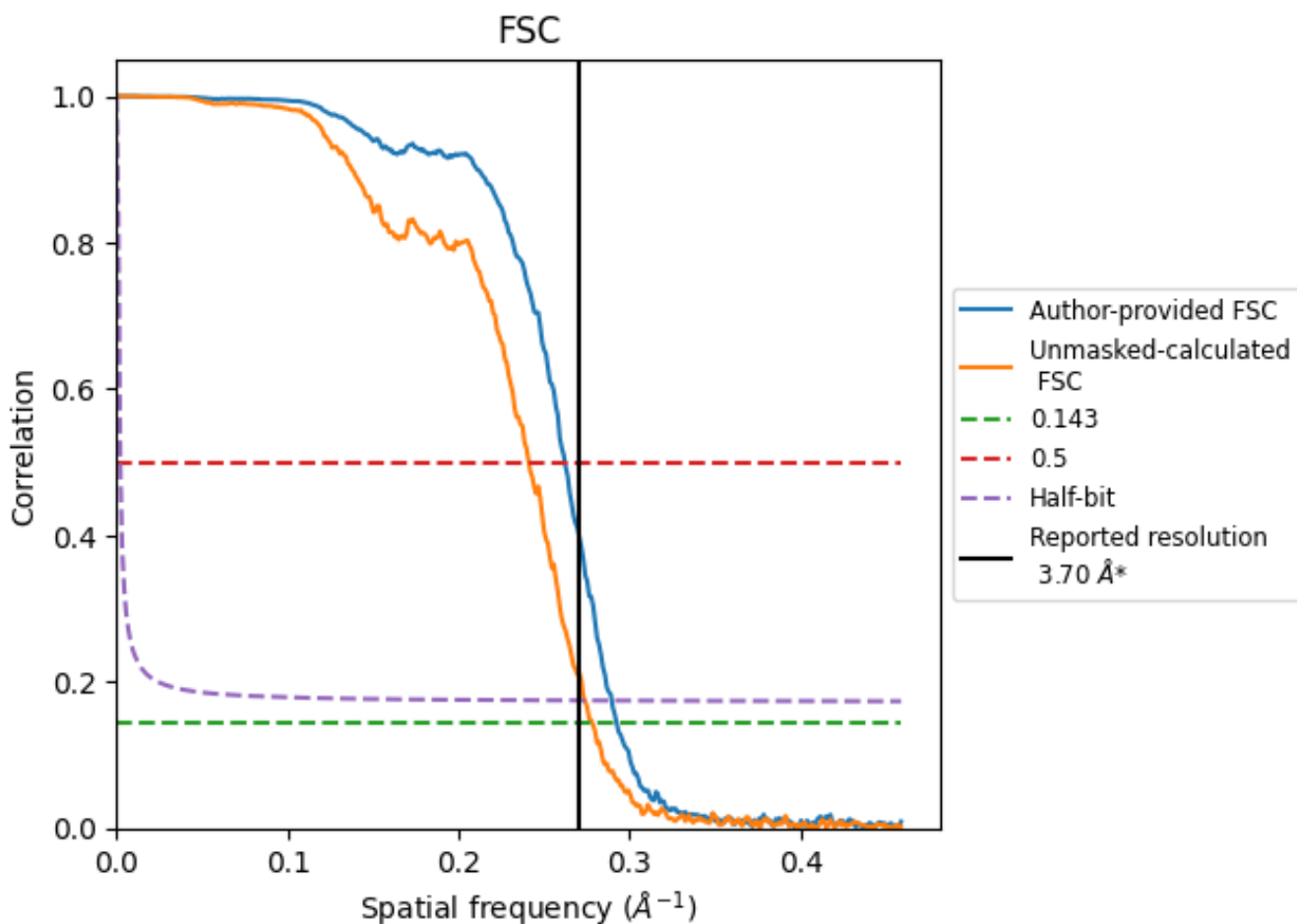


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.42	3.82	3.45
Unmasked-calculated*	3.59	4.15	3.65

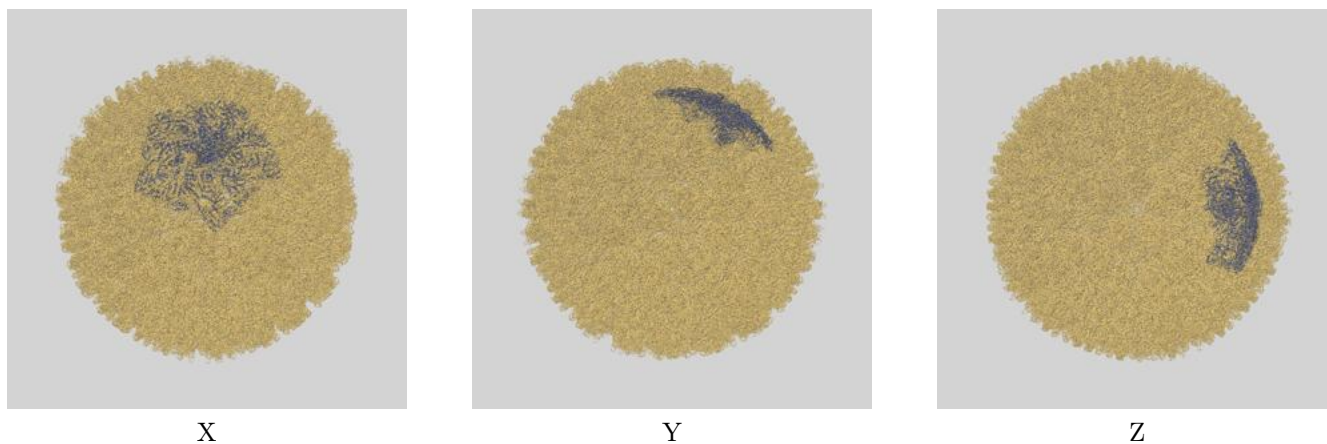
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

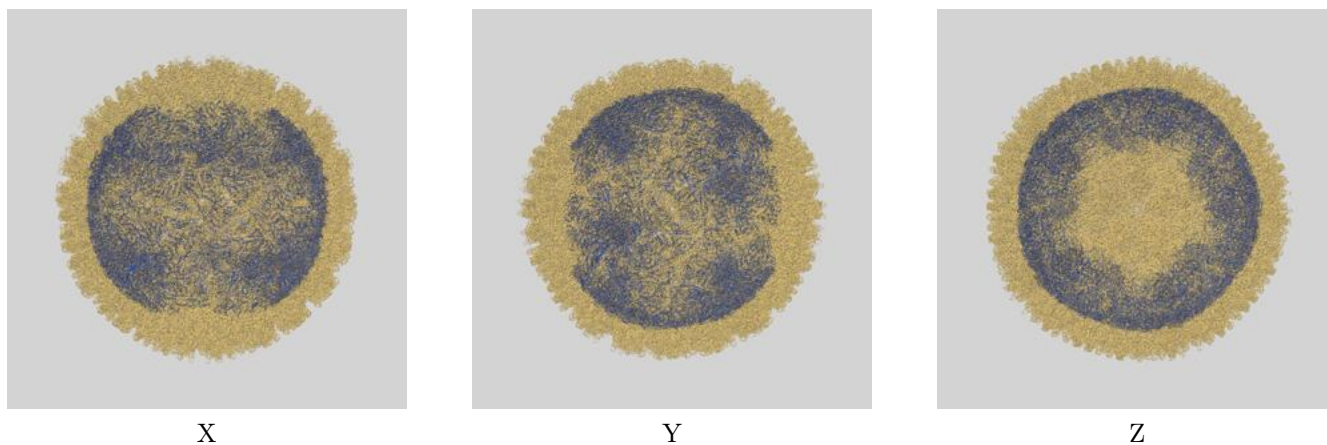
This section contains information regarding the fit between EMDB map EMD-33404 and PDB model 7XR3. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)



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



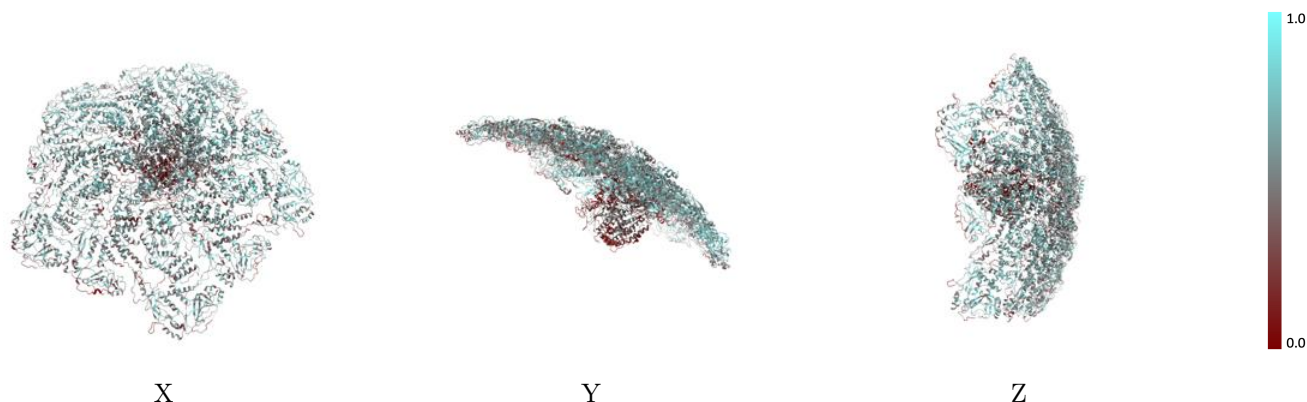
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

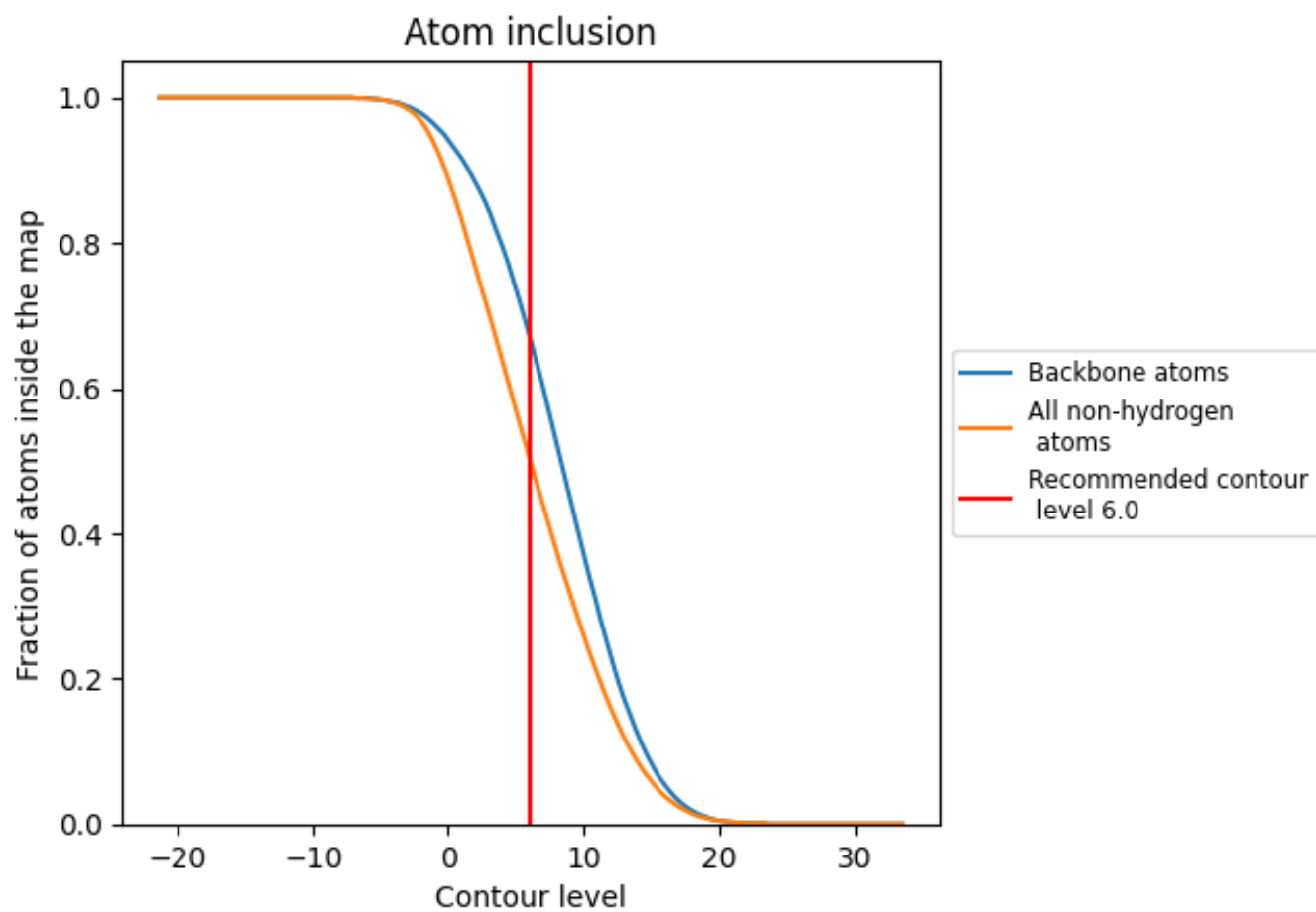
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (6.0).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5040	0.3580
A	0.5410	0.3990
B	0.5700	0.3920
C	0.5580	0.3950
D	0.5790	0.4090
E	0.5080	0.3430
F	0.5540	0.3670
G	0.4850	0.3300
H	0.5060	0.3160
I	0.5160	0.3590
J	0.5180	0.3340
Z	0.3130	0.3130

