



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 10:30 AM EST

PDB ID : 7LIV  
EMDB ID : EMD-23386  
Title : Structure of human transfer RNA visualized in the cytomegalovirus, a DNA virus  
Authors : Liu, Y.T.; Strugatsky, D.; Liu, W.; Zhou, Z.H.  
Deposited on : 2021-01-28  
Resolution : 3.60 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.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

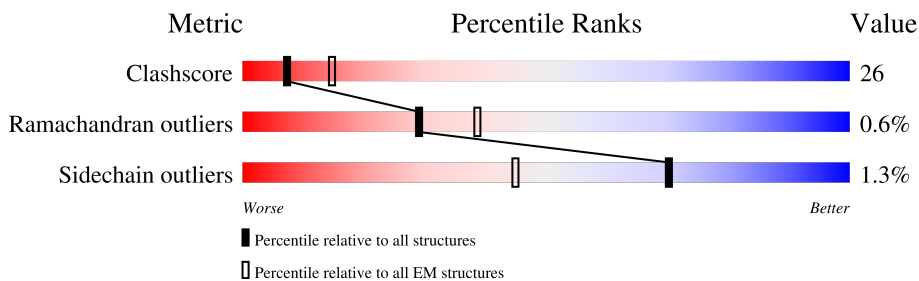
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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.




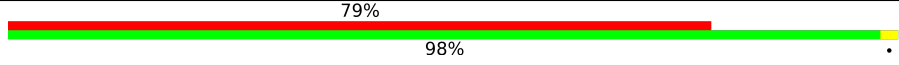

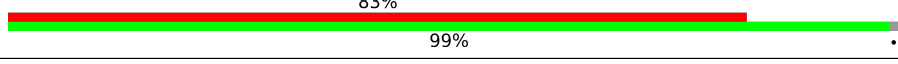
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1370	65% (Poor fit), 63% (0 outliers), 33% (1 outlier), 2% (2 outliers), 1% (3+ outliers), 1% (Not modelled)
1	C	1370	64% (Poor fit), 61% (0 outliers), 37% (1 outlier), 2% (2 outliers), 1% (3+ outliers), 1% (Not modelled)
1	J	1370	67% (Poor fit), 61% (0 outliers), 36% (1 outlier), 2% (2 outliers), 1% (3+ outliers), 1% (Not modelled)
2	4	285	94% (Poor fit), 67% (0 outliers), 32% (1 outlier), 2% (2 outliers), 1% (3+ outliers), 1% (Not modelled)
2	5	285	86% (Poor fit), 71% (0 outliers), 29% (1 outlier), 2% (2 outliers), 1% (3+ outliers), 1% (Not modelled)
2	6	285	80% (Poor fit), 68% (0 outliers), 32% (1 outlier), 2% (2 outliers), 1% (3+ outliers), 1% (Not modelled)
3	D	75	63% (Poor fit), 47% (0 outliers), 37% (1 outlier), 16% (2 outliers), 1% (3+ outliers), 1% (Not modelled)
3	E	75	65% (Poor fit), 59% (0 outliers), 25% (1 outlier), 16% (2 outliers), 1% (3+ outliers), 1% (Not modelled)

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Mol	Chain	Length	Quality of chain
3	Z	75	 <p>64% 56% 28% 16%</p>
4	p	290	 <p>79% 98%</p>
5	q	306	 <p>60% 78% 21%</p>
5	r	306	 <p>83% 99%</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 47058 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		
1	A	1328	Total	C	N	O	S	0	0
			10526	6706	1827	1934	59		
1	C	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		

- Molecule 2 is a protein called Tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	5	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
2	6	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
2	4	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

- Molecule 3 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Z	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	D	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
3	E	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	p	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

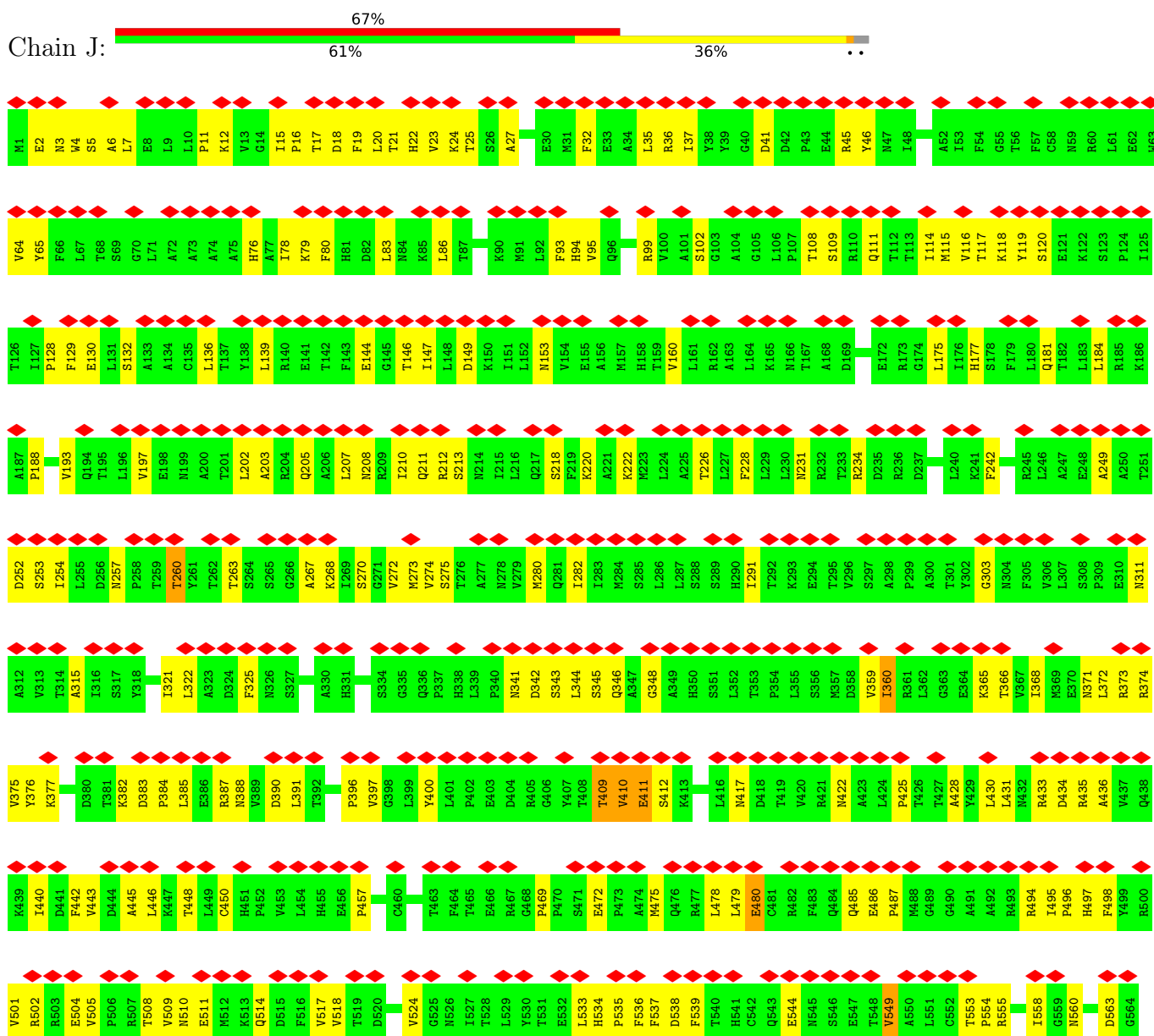
- Molecule 5 is a protein called Triplex capsid protein 2.

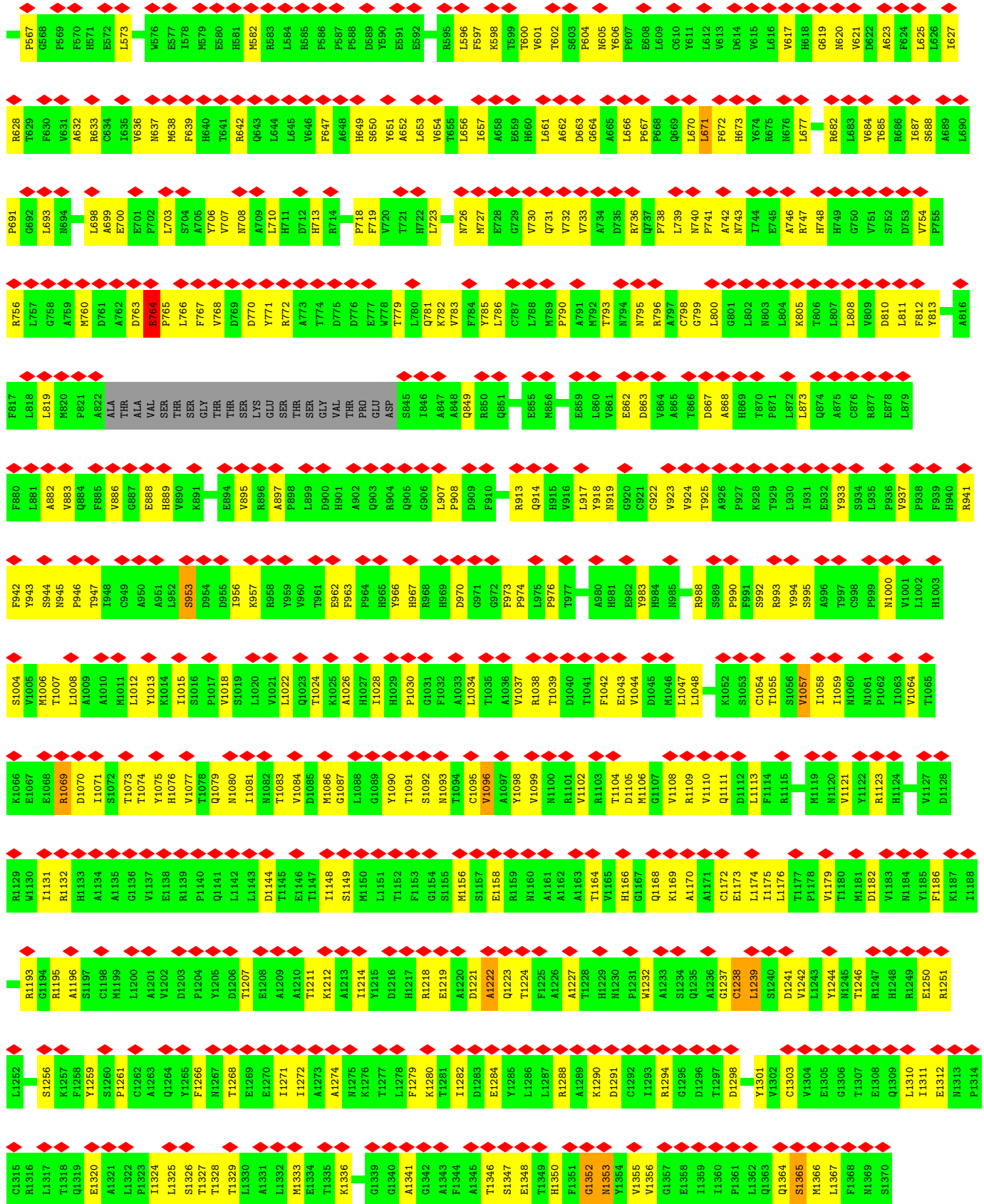
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	q	241	Total	C	N	O	S	0	0
			1911	1236	328	331	16		
5	r	304	Total	C	N	O	S	0	0
			2411	1544	420	429	18		

### 3 Residue-property plots

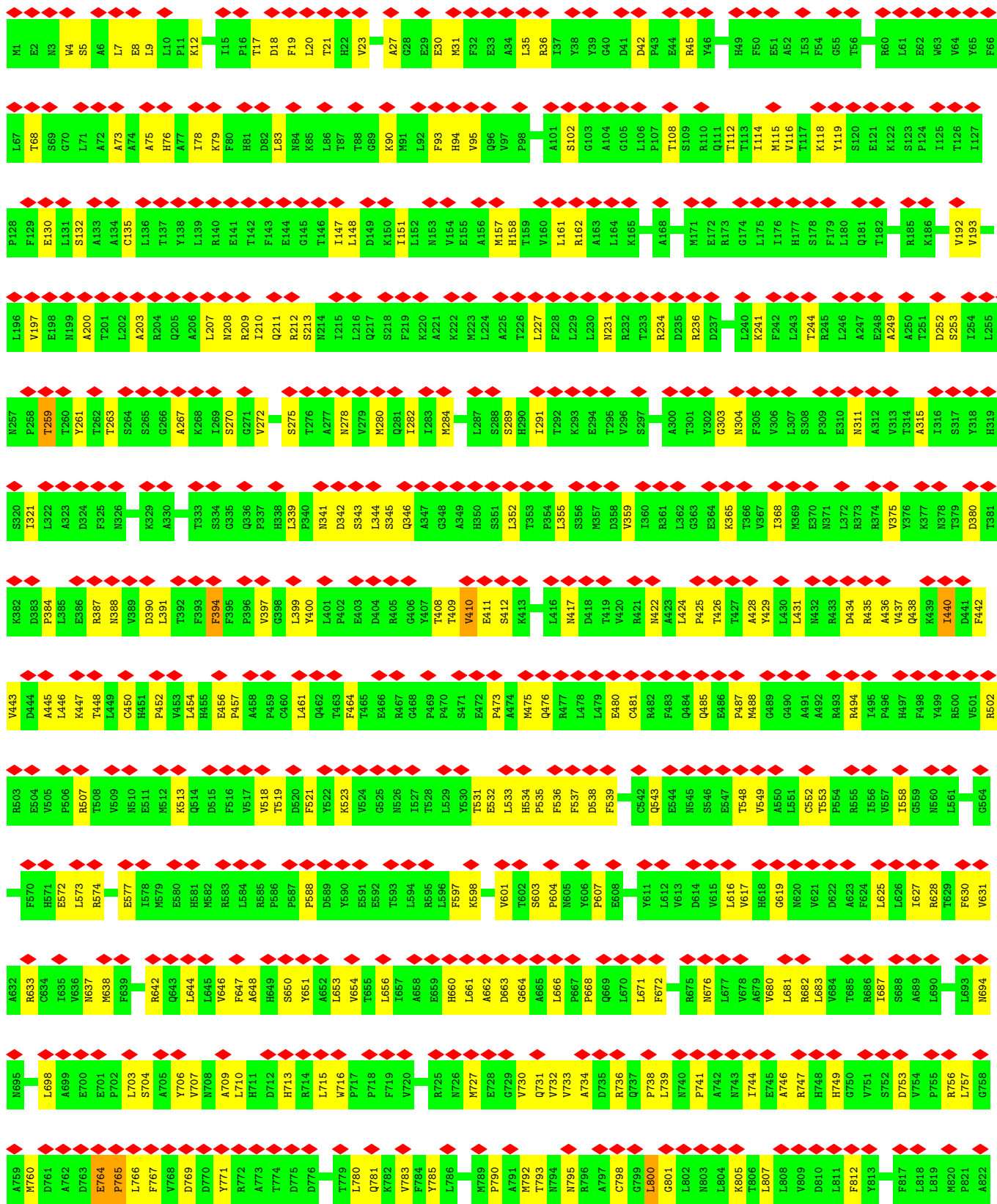
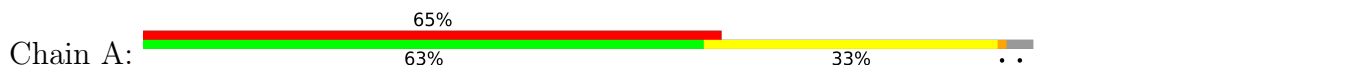
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

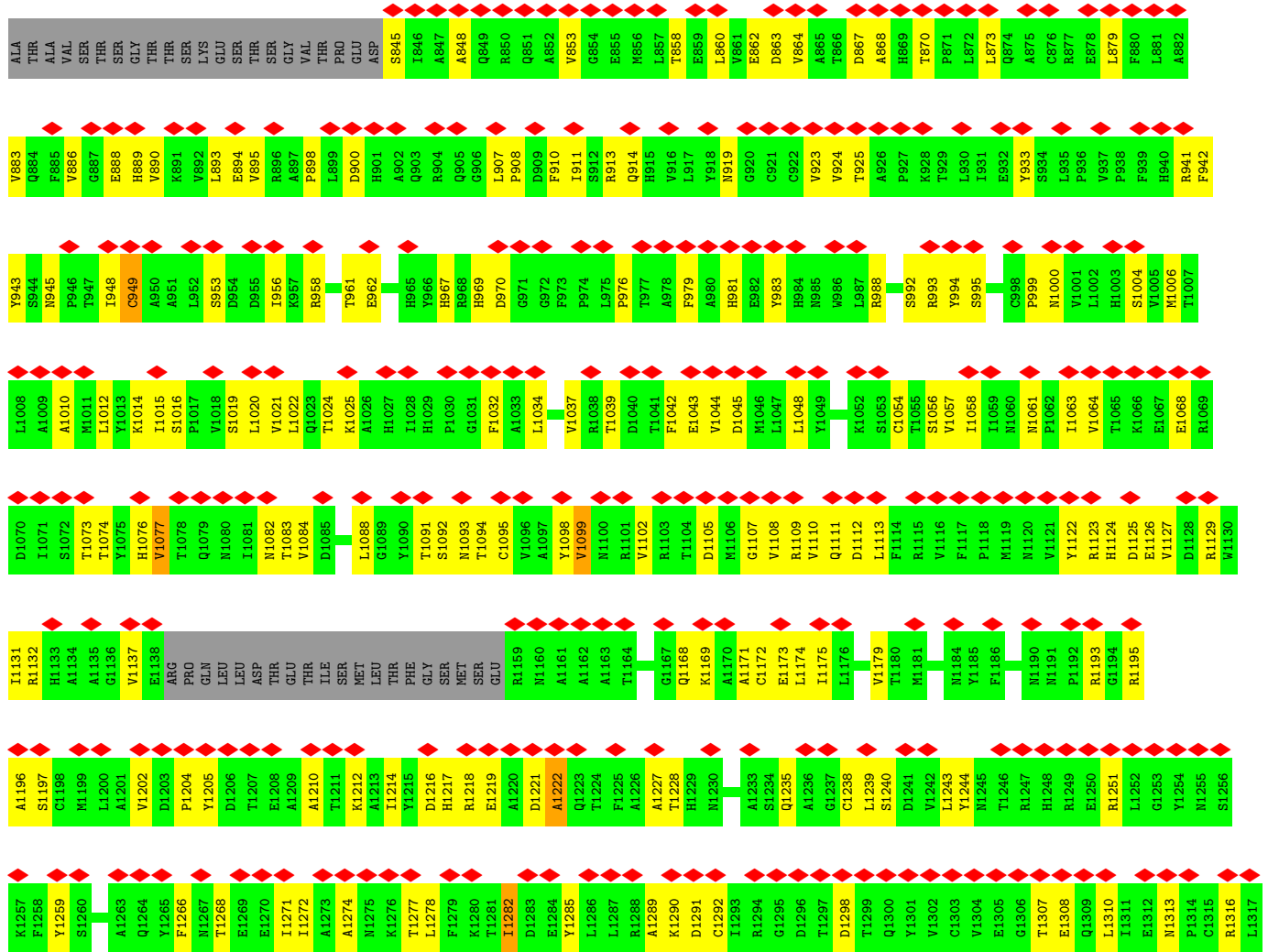




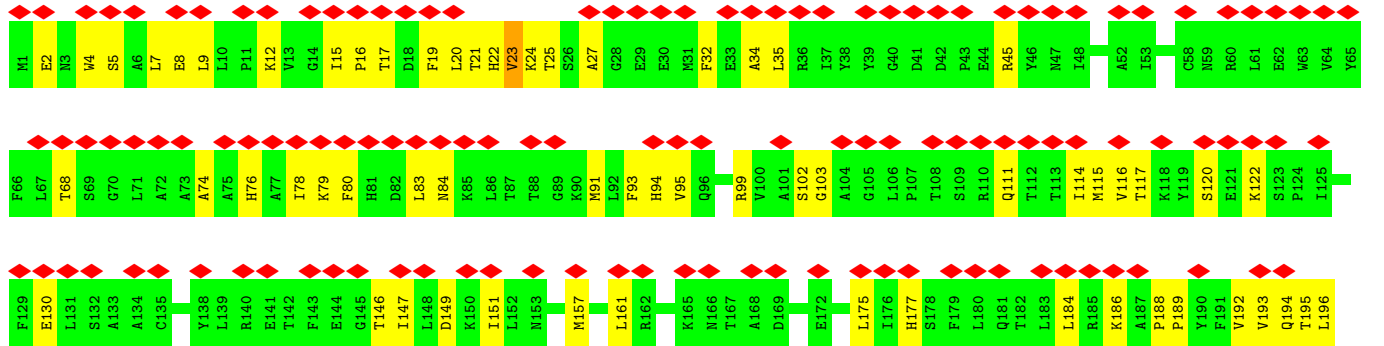
• Molecule 1: Major capsid protein



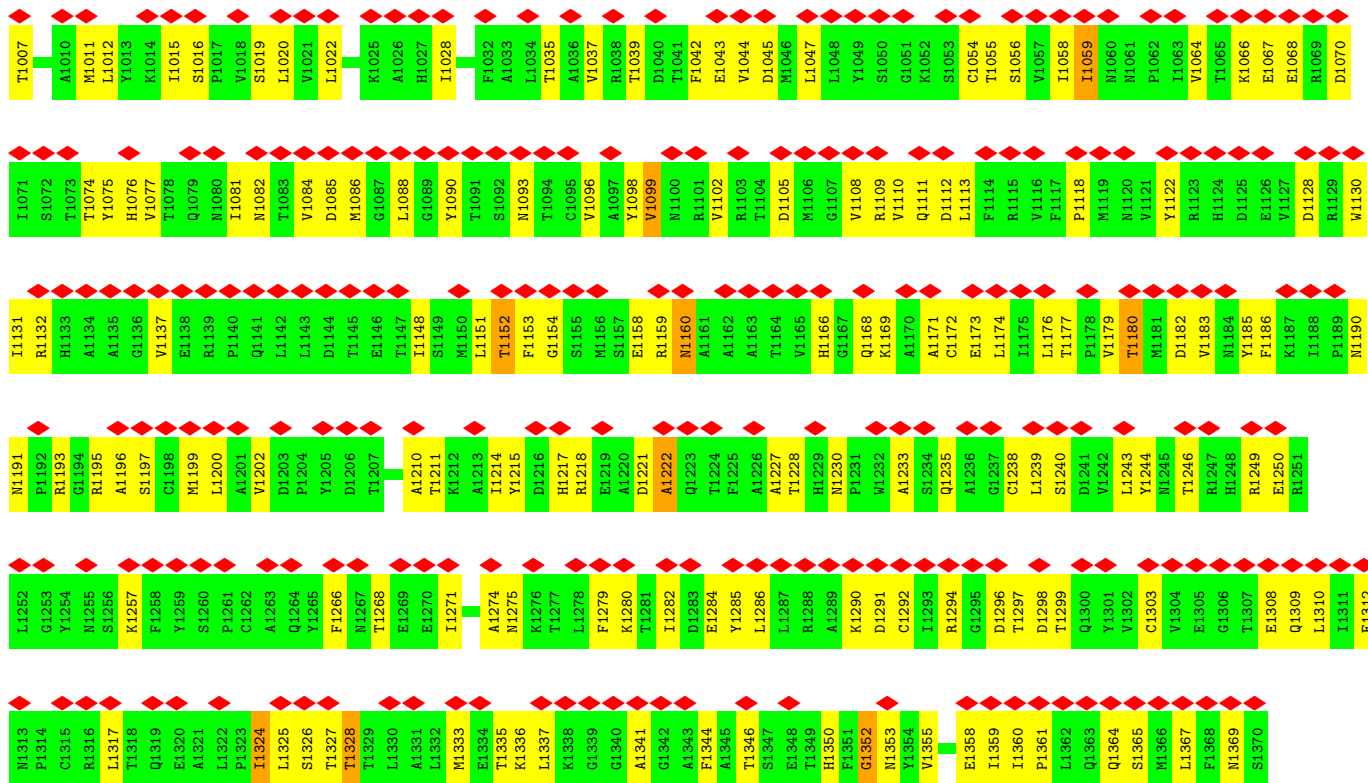




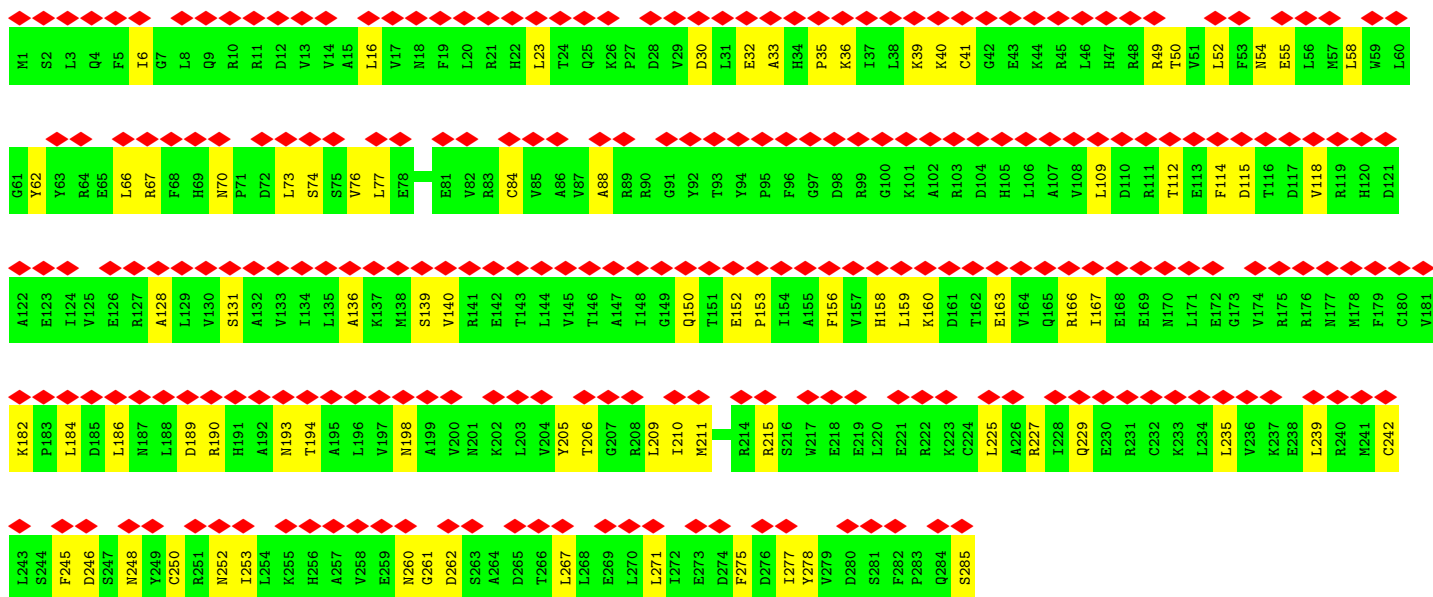
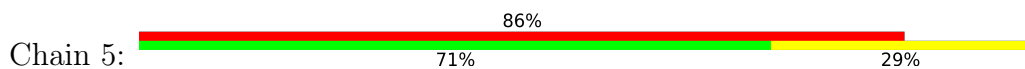
• Molecule 1: Major capsid protein



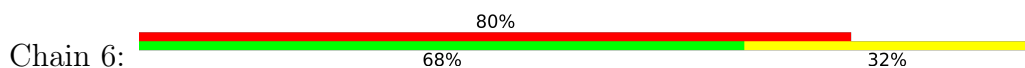
V197	E198	N199	A200	T201	A203	R204	Q205	A206	L207	N208	R209	I210	Q211	R212	I215	L216	Q217	S218	F219	K220	A221	K222	M223	L224	A225	T226	L227	F228	L229	L230	N231	R232	R234	D235	R236	D237	Y238	V239	L240	K241	F242	L243	T244	R245	L246	A247	E248	A249	A250	T251	D252	S253	I254	L255	D256	N257																																																												
P258	T259	T260	Y261	T262	T263	S264	S265	G266	A267	K268	I269	S270	M273	V274	S275	T276	A277	N278	V279	M280	Q281	I282	I283	M284	S285	L286	L287	S288	S289	H290	I291	T292	K293	E294	T295	V296	S297	A298	P299	A300	T301	Y302	G303	N304	F305	V306	L307	S308	P309	E310	M311	A312	V313	T314	A315	S316	Y317	Y318																																																										
H319	I321	L322	A323	D324	F325	N326	S327	Y328	K329	A330	H331	L332	T333	S334	G335	Q336	P337	H338	L339	P340	N341	D342	I343	S344	S345	Q346	A347	G348	A349	H350	S351	L352	T353	P354	L355	S356	M357	D358	V359	I360	R361	L362	G363	E364	K365	T366	V367	L368	M369	E370	N371	L372	R373	R374	V375	K377	N378																																																											
T379	D380	T381	K382	D383	P384	L385	E386	R387	N388	D389	L391	T392	F395	P396	G398	L399	Y400	L401	P402	E403	D404	R405	T408	T409	V410	E411	S412	K413	V414	K415	L416	M417	D418	T419	V420	R421	N422	A423	L424	P425	T426	T427	A428	Y429	L430	L431	M432	R433	D434	R435	A436	V437	Q438	K439	T440																																																													
D441	F442	V443	A445	L446	K447	T448	L449	C450	H451	L454	H455	E456	P457	A458	P459	C460	L461	Q462	T463	F464	T465	E466	R467	G468	P469	P470	S471	E472	F473	A474	M475	Q476	R477	L478	L479	E480	C481	R482	F483	Q484	Q485	E486	P487	M488	C489	G490	A491	A492	R493	R494	T495	P496	H497	F498	Y499	R500	V501																																																											
R502	R503	E504	R507	T508	V509	N510	K513	Q514	D515	V518	T519	D520	F521	Y522	K523	V524	G525	N526	L529	E532	L533	H534	P535	F536	F537	D538	F539	T540	H541	C542	Q543	E544	E545	S546	E547	T548	V549	A550	L551	C552	T553	P554	R555	L556	V557	L558	L561	P562	D563	G564	L565	L566	A566	P567																																																														
E572	L573	R574	E577	L578	M579	E580	H581	H582	R583	L584	R585	P586	F587	P588	D589	Y590	E591	E592	T593	L594	R595	L596	F597	K598	T599	T600	V601	T602	S603	P604	M605	V606	P607	E608	L609	G610	Y611	L612	V613	D614	V615	L616	V617	H618	G619	M620	V621	D622	A623	F624	L625	D626	L627	R628	T629	F630	V631																																																											
A632	R633	C634	L635	V636	M637	M638	F639	H640	R642	Q643	L644	L645	V646	F647	A648	Y651	A652	L653	V654	T655	L656	L657	A658	E659	H660	L661	A662	D663	L666	P667	P668	L669	L670	L671	F672	H673	V674	R675	L739	M740	P741	A742	N743	L744	L745	A746	R747	H748	H749	G750	V751	S752	D753	R756	A759	M760																																																												
G696	D697	L698	A699	E700	E701	F702	L703	S704	T641	A705	Y706	Y707	L710	H711	D712	H713	R714	L715	W716	F717	F718	F719	H722	R725	N726	M727	E728	G729	W730	Q731	V732	V733	A734	D735	R736	Q737	F738	L739	N740	P741	A742	N743	L744	L745	A746	R747	H748	H749	G750	V751	S752	D753	R756	A759	M760																																																													
D761	A762	D763	E764	F765	L766	F767	V768	D769	D770	Y771	R772	D775	D776	E777	L780	Q781	K782	V783	F784	Y785	L786	C787	L788	M789	P790	A791	N792	T793	N794	N795	R796	A797	C798	G799	L800	C801	L802	M803	L804	K805	T806	L807	L808	H809	D810	L811	F812	Y813	R814	F815	A816	F817	L818	L819	M820	P821	A822																																																											
ALA	THR	ALA	VAL	SER	THR	SER	GLY	THR	THR	SER	LYS	GLU	SER	THR	SER	GLY	VAL	THR	PRO	GLU	ASP	ASP	ASP	Q849	R850	Q851	W853	G854	E855	M856	L857	T858	E859	L860	N861	D862	D863	W864	A865	T866	D867	A868	H869	T870	F871	L872	L873	Q874	A875	C876	R877	E878	L879	F880	L881	A882	H883	Q884	F885	V886	E888	H889	K891	V892	L893	E894	V895	R896	A897	P898	L899	D900	H901	A902	Q903	R904	Q905	G906	L907	P908	D909	F910	I911	S912	R913	Q914	H915	V916	L917	Y918	N919	G920	C921	C922	V923	Y924	T925	A926	P927	K928	T929	L930	I931	E932	Y933	S934	L935	P936	N1000	V1001	L1002	H1003	S1004	V1005	M1006	Y943

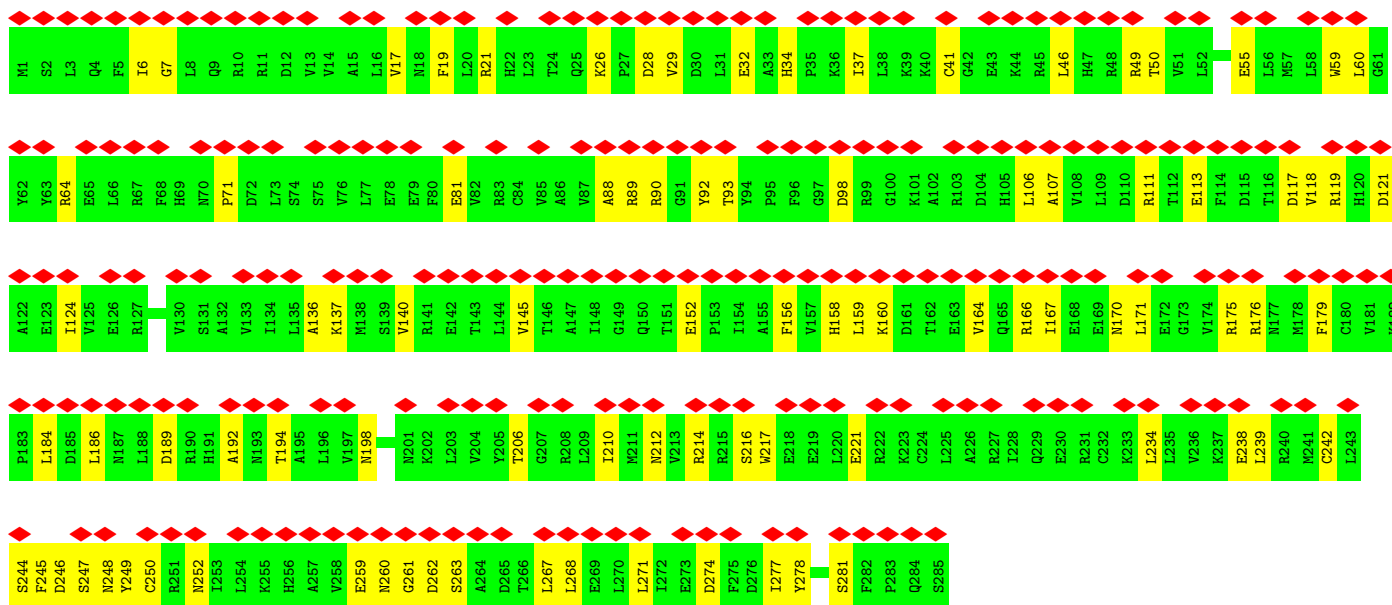


• Molecule 2: Tegument protein pp150

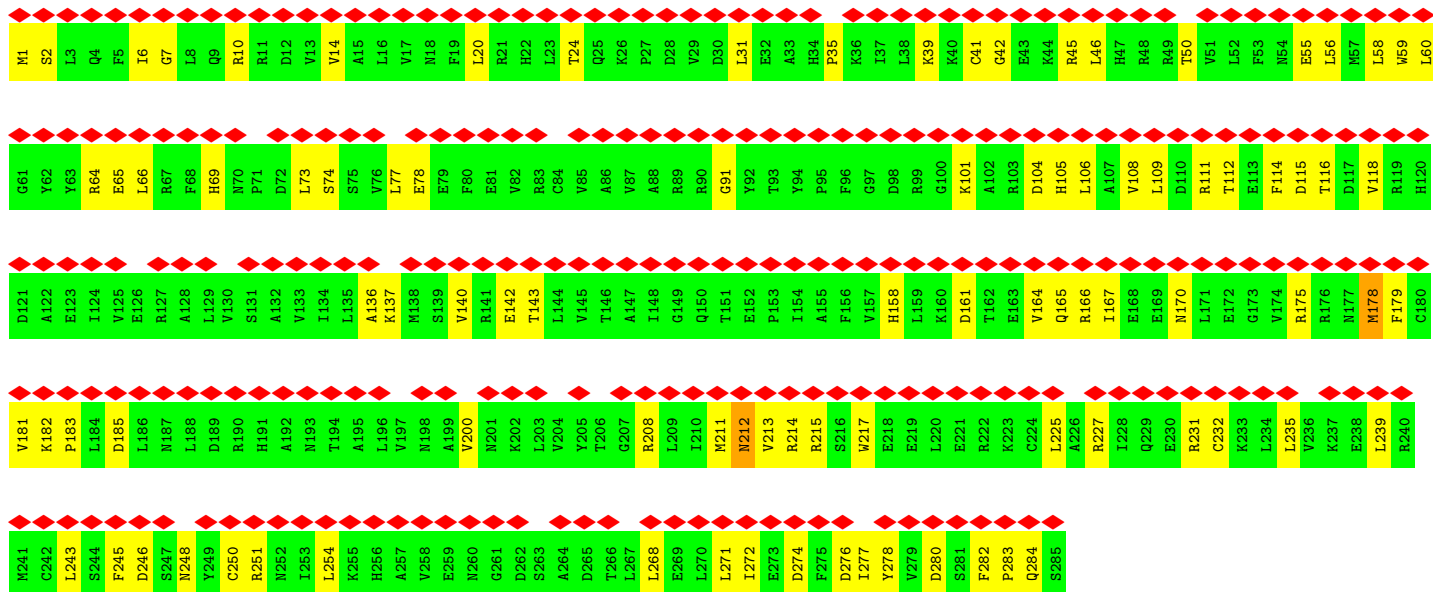
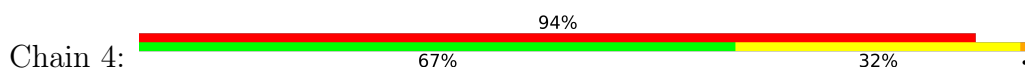


• Molecule 2: Tegument protein pp150

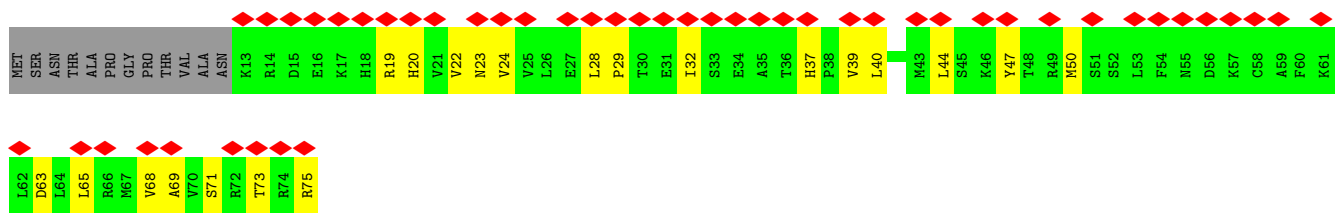




• Molecule 2: Tegument protein pp150



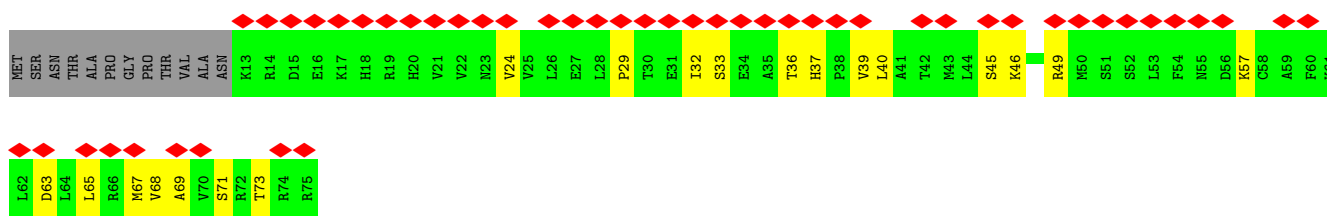
• Molecule 3: Small capsomere-interacting protein



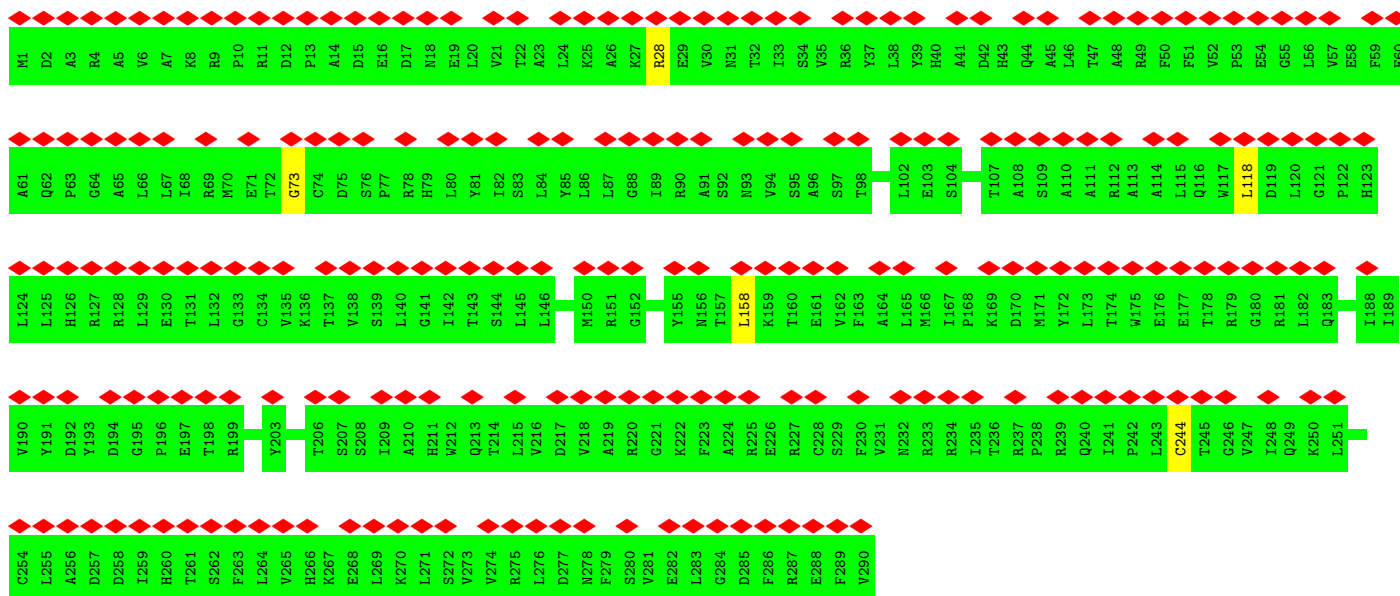
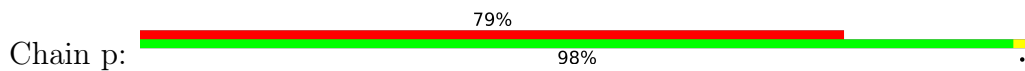
• Molecule 3: Small capsomere-interacting protein



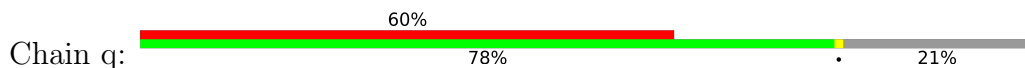
• Molecule 3: Small capsomere-interacting protein

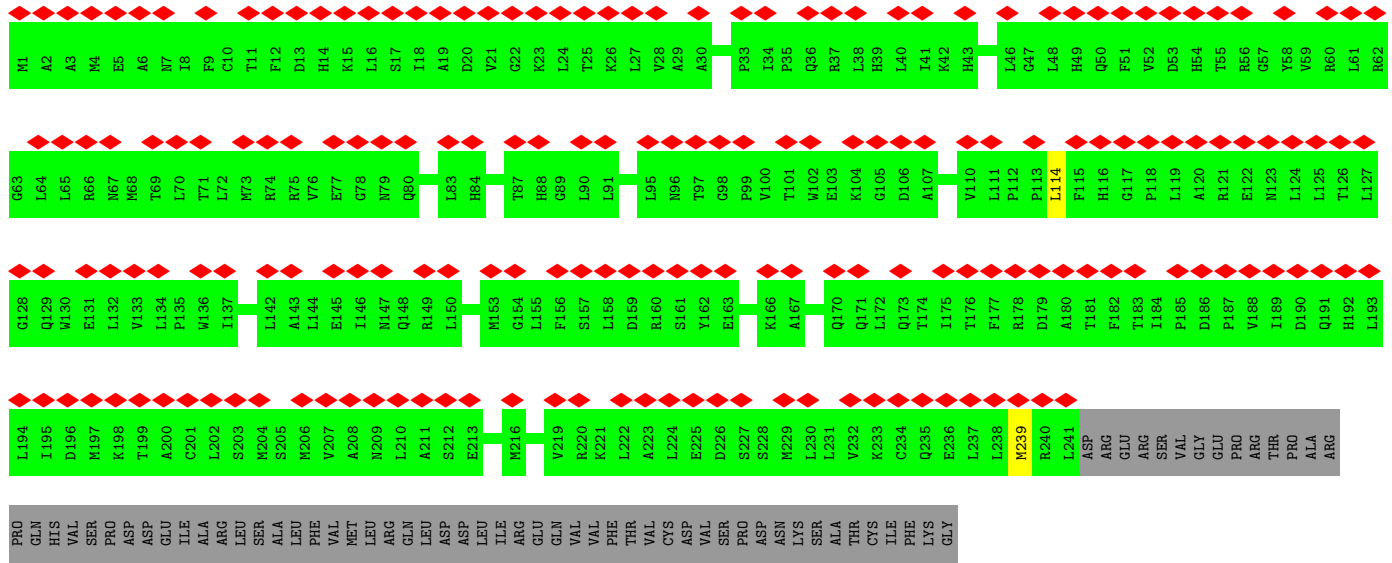


• Molecule 4: Triplex capsid protein 1

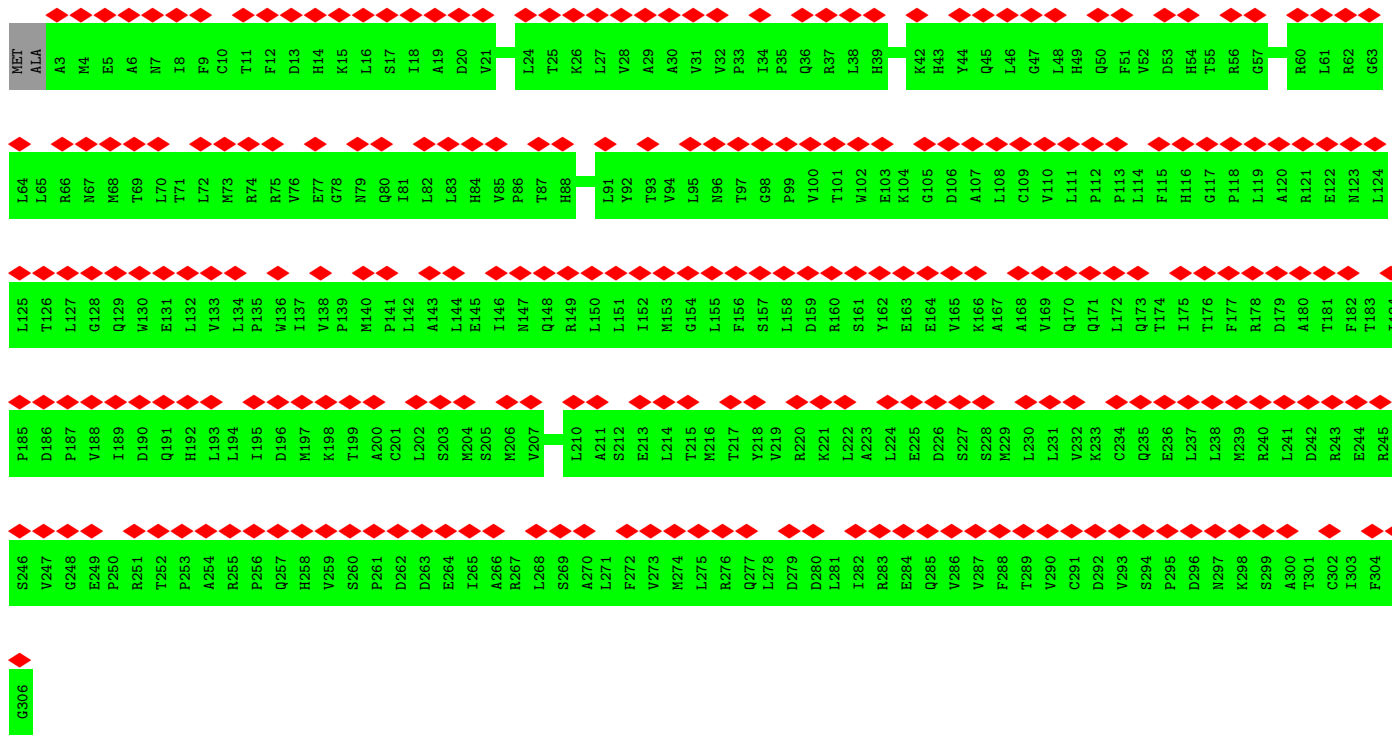
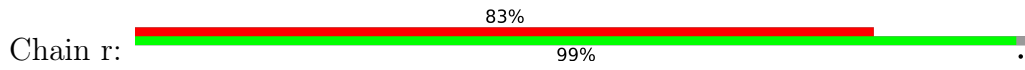


• Molecule 5: Triplex capsid protein 2





• Molecule 5: Triplex capsid protein 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97166	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 ( $e^-/\text{\AA}^2$ )	18.9	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	0.083	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	412.16, 412.16, 412.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.61, 1.61, 1.61	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	0.48	0/10779	0.56	0/14684
1	C	0.49	0/10937	0.56	0/14899
1	J	0.48	0/10937	0.56	0/14899
2	4	0.38	0/2366	0.51	0/3192
2	5	0.36	0/2366	0.49	0/3192
2	6	0.40	0/2366	0.51	0/3192
3	D	0.42	0/520	0.50	0/697
3	E	0.41	0/520	0.57	0/697
3	Z	0.41	0/520	0.53	0/697
4	p	0.42	0/2374	0.57	0/3221
5	q	0.39	0/1949	0.55	0/2649
5	r	0.40	0/2458	0.59	0/3339
All	All	0.46	0/48092	0.55	0/65358

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](#)

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	10526	0	10468	605	0
1	C	10681	0	10620	681	0
1	J	10681	0	10618	630	0
2	4	2328	0	2363	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5	2328	0	2363	70	0
2	6	2328	0	2363	81	0
3	D	513	0	539	56	0
3	E	513	0	539	26	0
3	Z	513	0	539	33	0
4	p	2325	0	2362	0	0
5	q	1911	0	2007	0	0
5	r	2411	0	2500	0	0
All	All	47058	0	47281	2125	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 26.

The worst 5 of 2125 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)
1:C:203:ALA:CB	1:C:207:LEU:HD21	1.30	1.60
1:A:207:LEU:CD1	1:A:212:ARG:HG3	1.38	1.53
1:C:19:PHE:CE1	1:C:23:VAL:N	1.78	1.51
1:J:440:ILE:CD1	1:J:1108:VAL:HG11	1.38	1.50
1:A:207:LEU:HD11	1:A:212:ARG:CG	1.39	1.49

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	1322/1370 (96%)	1242 (94%)	73 (6%)	7 (0%)	29 68
1	C	1344/1370 (98%)	1255 (93%)	78 (6%)	11 (1%)	19 59
1	J	1344/1370 (98%)	1262 (94%)	71 (5%)	11 (1%)	19 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4	283/285 (99%)	273 (96%)	10 (4%)	0	100	100
2	5	283/285 (99%)	271 (96%)	11 (4%)	1 (0%)	34	71
2	6	283/285 (99%)	274 (97%)	8 (3%)	1 (0%)	34	71
3	D	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
3	E	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
3	Z	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
4	p	288/290 (99%)	273 (95%)	13 (4%)	2 (1%)	22	61
5	q	239/306 (78%)	231 (97%)	7 (3%)	1 (0%)	34	71
5	r	302/306 (99%)	288 (95%)	14 (5%)	0	100	100
All	All	5871/6092 (96%)	5548 (94%)	289 (5%)	34 (1%)	29	64

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	409	THR
1	J	410	VAL
1	J	764	GLU
1	J	1070	ASP
1	J	1238	CYS

### 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	1155/1192 (97%)	1137 (98%)	18 (2%)	62	83
1	C	1174/1192 (98%)	1156 (98%)	18 (2%)	65	84
1	J	1174/1192 (98%)	1149 (98%)	25 (2%)	53	78
2	4	256/257 (100%)	254 (99%)	2 (1%)	81	91
2	5	256/257 (100%)	255 (100%)	1 (0%)	91	97
2	6	256/257 (100%)	256 (100%)	0	100	100
3	D	59/68 (87%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	59/68 (87%)	59 (100%)	0	100	100
3	Z	59/68 (87%)	59 (100%)	0	100	100
4	p	252/252 (100%)	249 (99%)	3 (1%)	71	87
5	q	214/273 (78%)	213 (100%)	1 (0%)	88	95
5	r	272/273 (100%)	272 (100%)	0	100	100
All	All	5186/5349 (97%)	5118 (99%)	68 (1%)	70	86

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1292	CYS
1	C	1324	ILE
4	p	118	LEU
1	J	1365	SER
1	J	1353	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	901	HIS
2	5	34	HIS
1	C	914	GLN
1	C	1160	ASN
2	6	170	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.

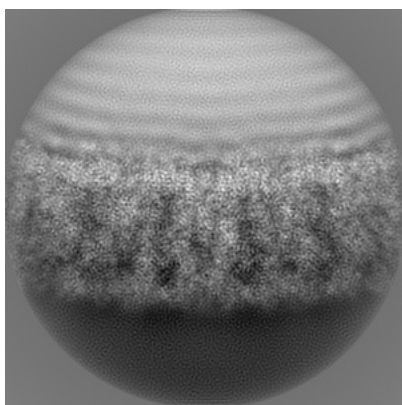
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23386. These allow visual inspection of the internal detail of the map and identification of artifacts.

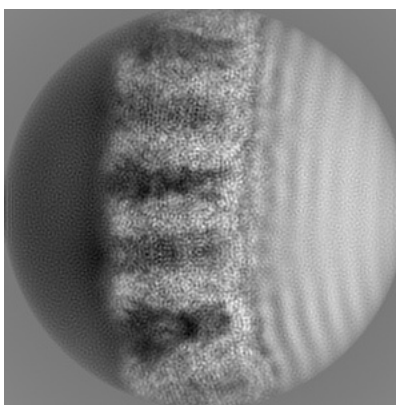
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

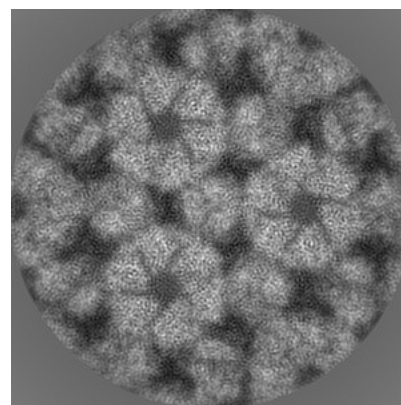
#### 6.1.1 Primary map



X



Y

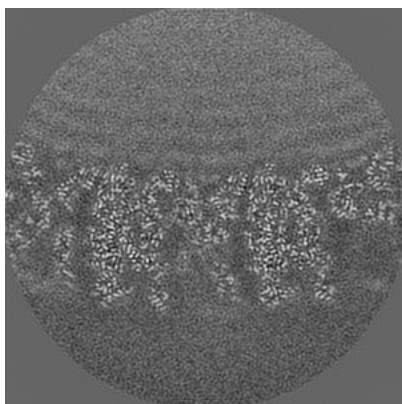


Z

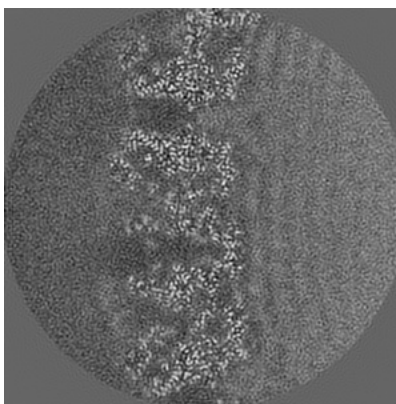
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

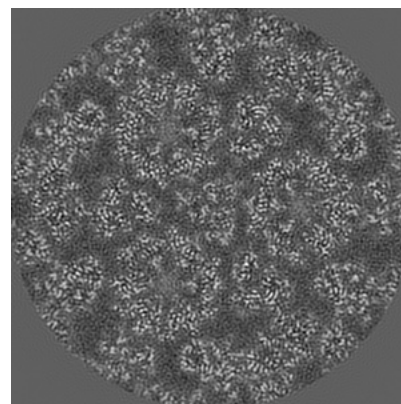
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

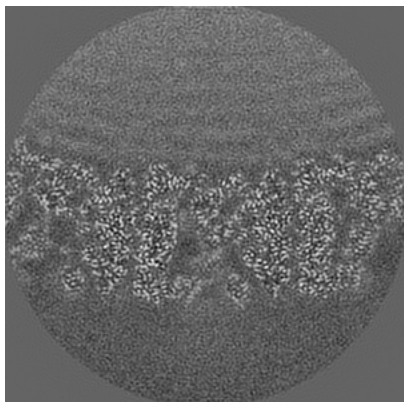


Z Index: 128

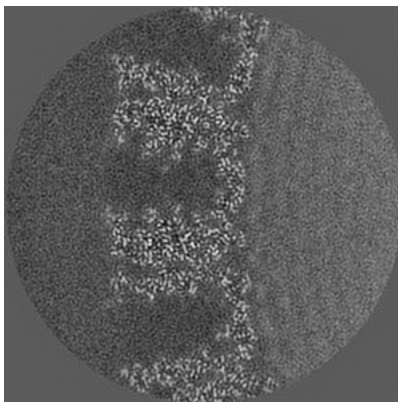
The images above show central slices of the map in three orthogonal directions.

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

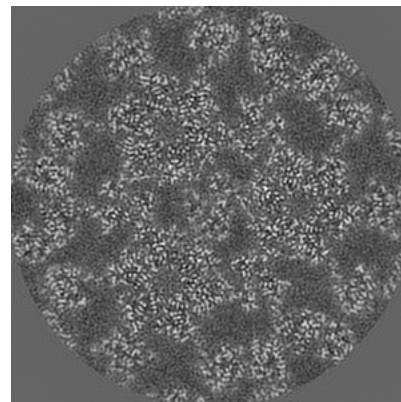
### 6.3.1 Primary map



X Index: 119



Y Index: 153



Z Index: 121

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

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

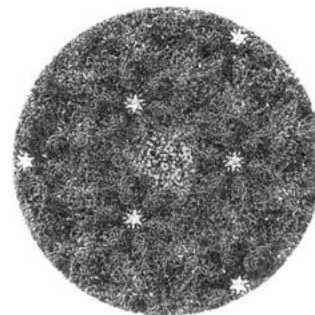
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

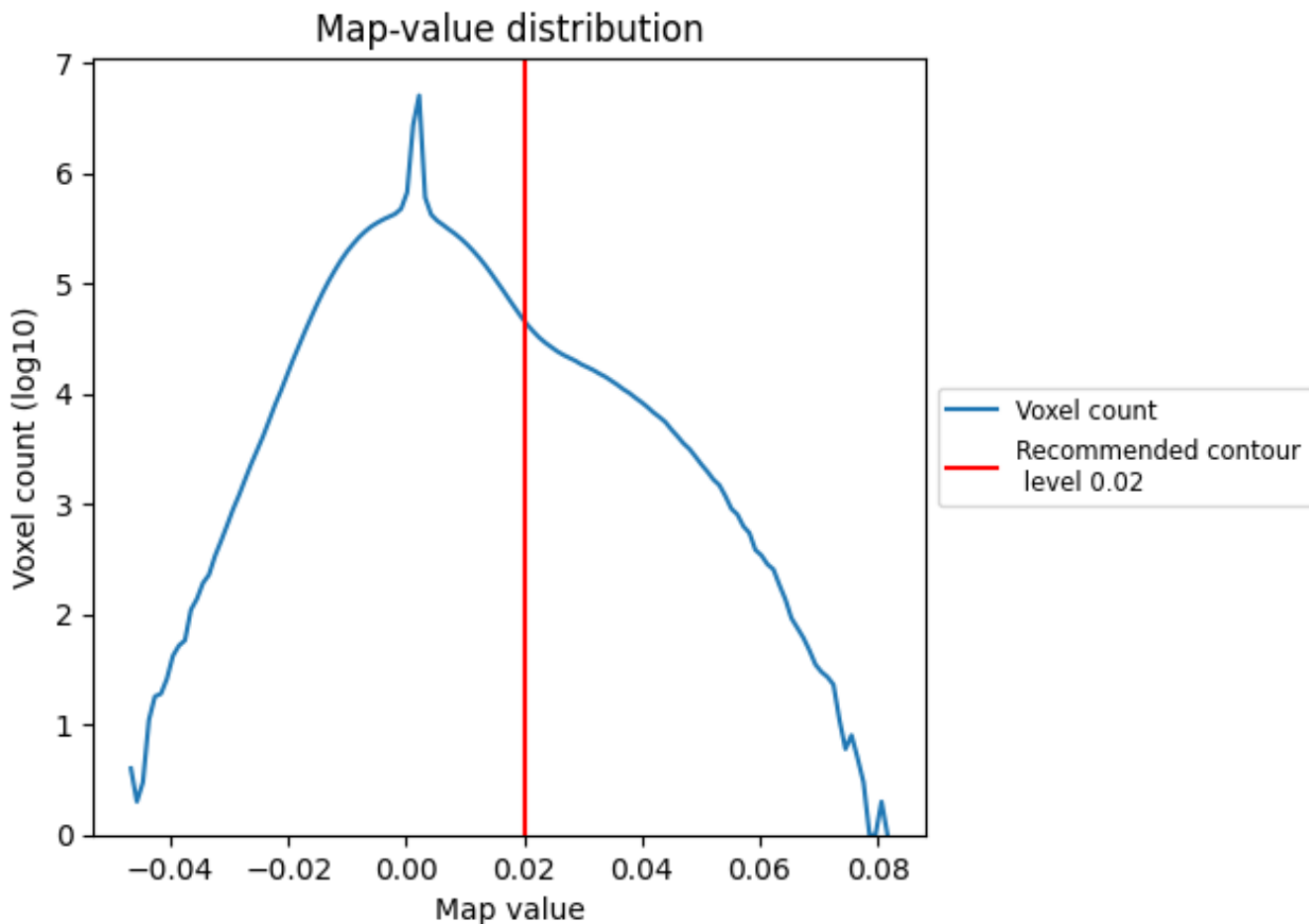
## 6.5 Mask visualisation

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.

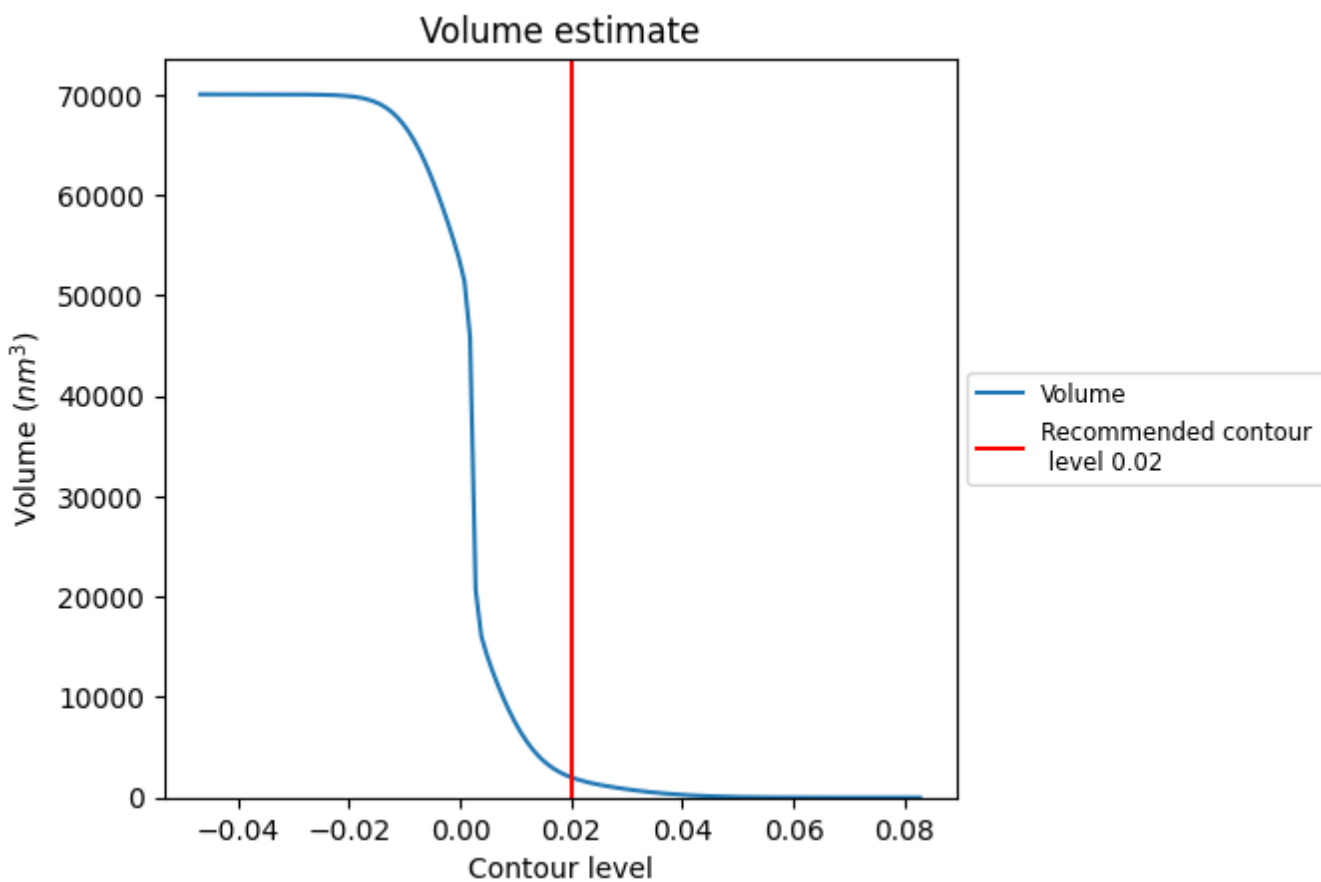
### 7.1 Map-value distribution [i](#)



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.



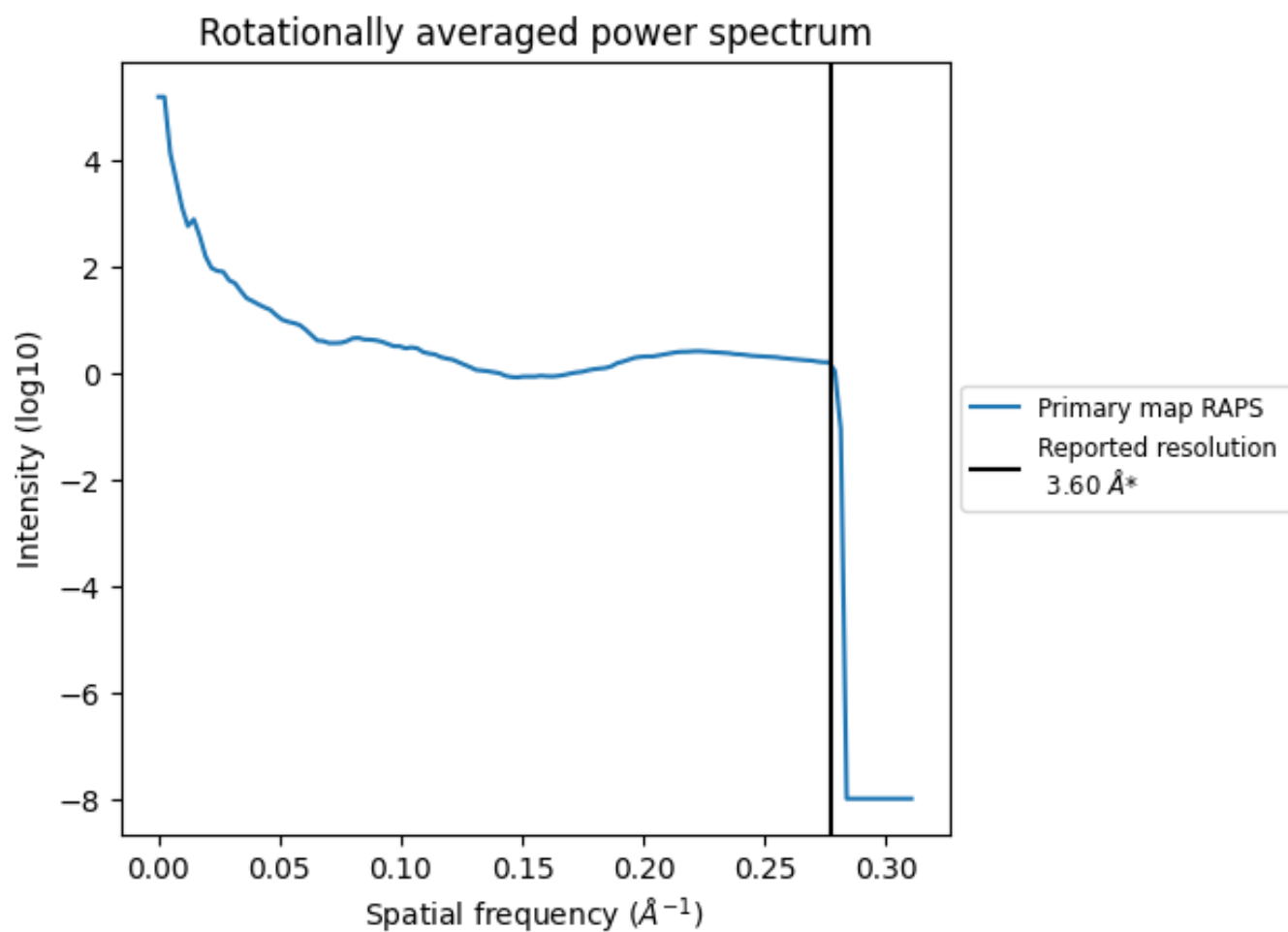
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2015 nm<sup>3</sup>; this corresponds to an approximate mass of 1820 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 0.278 Å<sup>-1</sup>

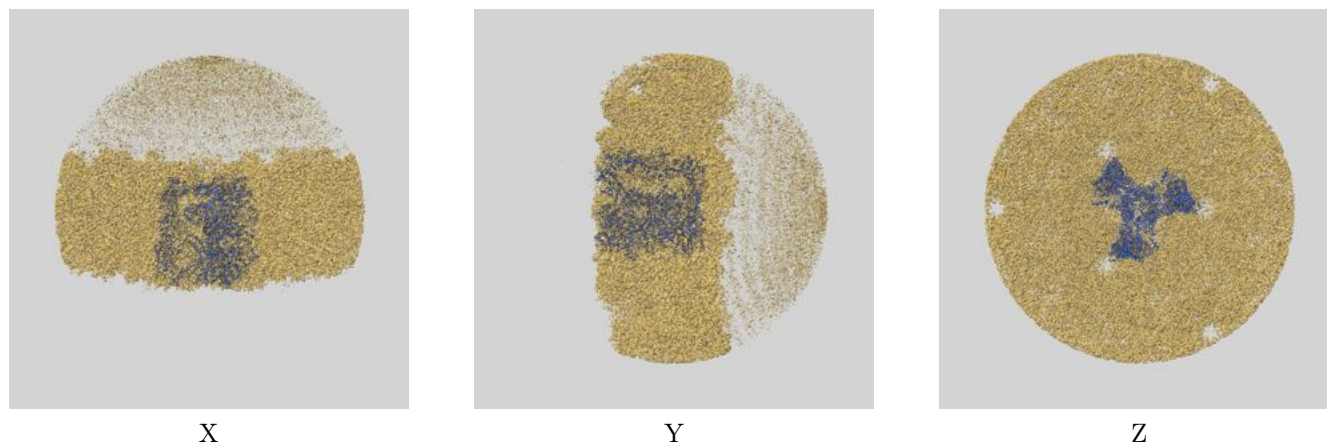
## 8 Fourier-Shell correlation

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

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

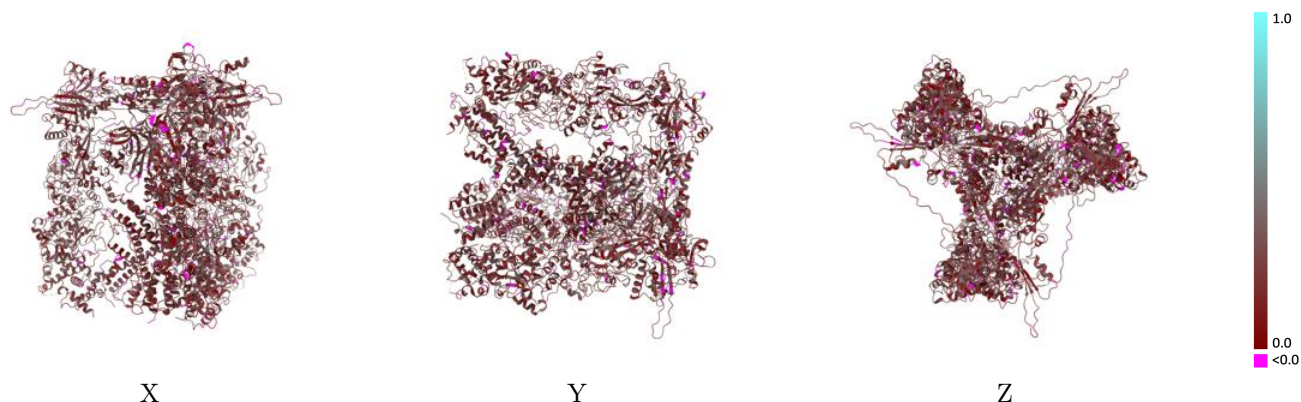
This section contains information regarding the fit between EMDB map EMD-23386 and PDB model 7LIV. Per-residue inclusion information can be found in section 3 on page 6.

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



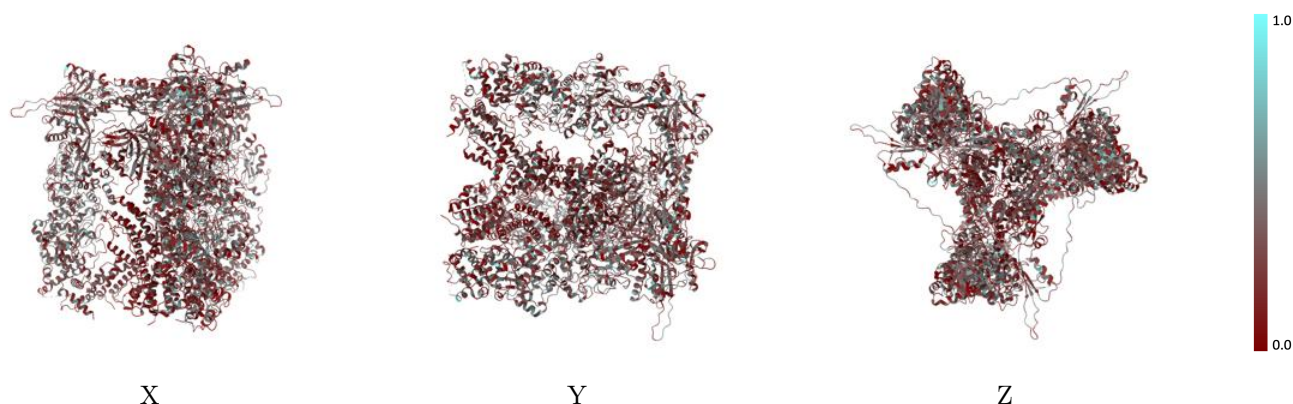
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



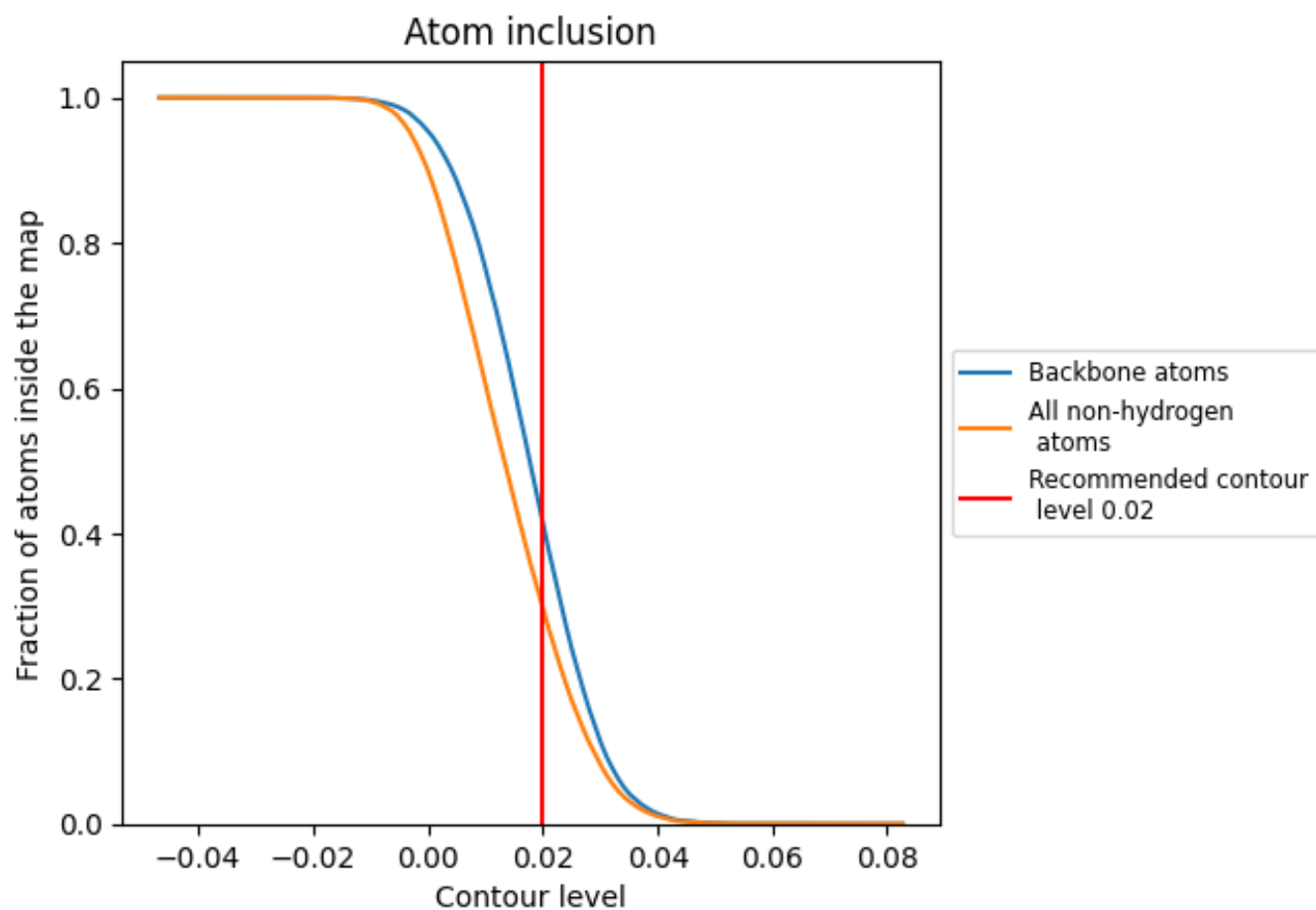
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 42% of all backbone atoms, 30% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2976	0.2310
4	0.1420	0.2040
5	0.1787	0.2130
6	0.2366	0.2360
A	0.3338	0.2400
C	0.3416	0.2380
D	0.2550	0.2280
E	0.2711	0.2290
J	0.3306	0.2290
Z	0.2570	0.2250
p	0.2283	0.2260
q	0.2696	0.2350
r	0.2319	0.2150

