



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 11:00 AM EST

PDB ID : 6PO2
EMDB ID : EMD-20407
Title : In situ structure of BTV RNA-dependent RNA polymerase in BTV core
Authors : He, Y.; Shivakoti, S.; Ding, K.; Cui, Y.; Roy, P.; Zhou, Z.H.
Deposited on : 2019-07-03
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

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

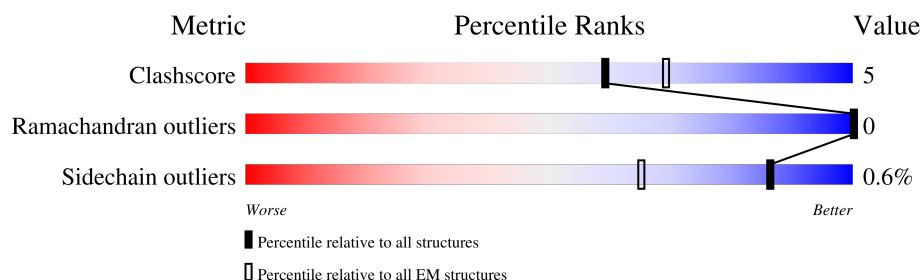
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 ≥ 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	1302	<div> <div>61%</div> <div>80%</div> <div>15%</div> <div>.</div> </div>
2	B	901	<div> <div>27%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
2	C	901	<div> <div>52%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	D	901	<div> <div>30%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
2	E	901	<div> <div>52%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	F	901	<div> <div>31%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	G	901	<div> <div>53%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	H	901	<div> <div>30%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	901	<div><div></div><div>51%</div><div></div><div>86%</div><div></div><div>12%</div><div></div><div></div></div>
2	J	901	<div><div></div><div>29%</div><div></div><div>85%</div><div></div><div>12%</div><div></div><div></div></div>
2	K	901	<div><div></div><div>51%</div><div></div><div>88%</div><div></div><div>10%</div><div></div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 80873 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1244	Total	C	N	O	S	0	0
			10062	6417	1720	1865	60		

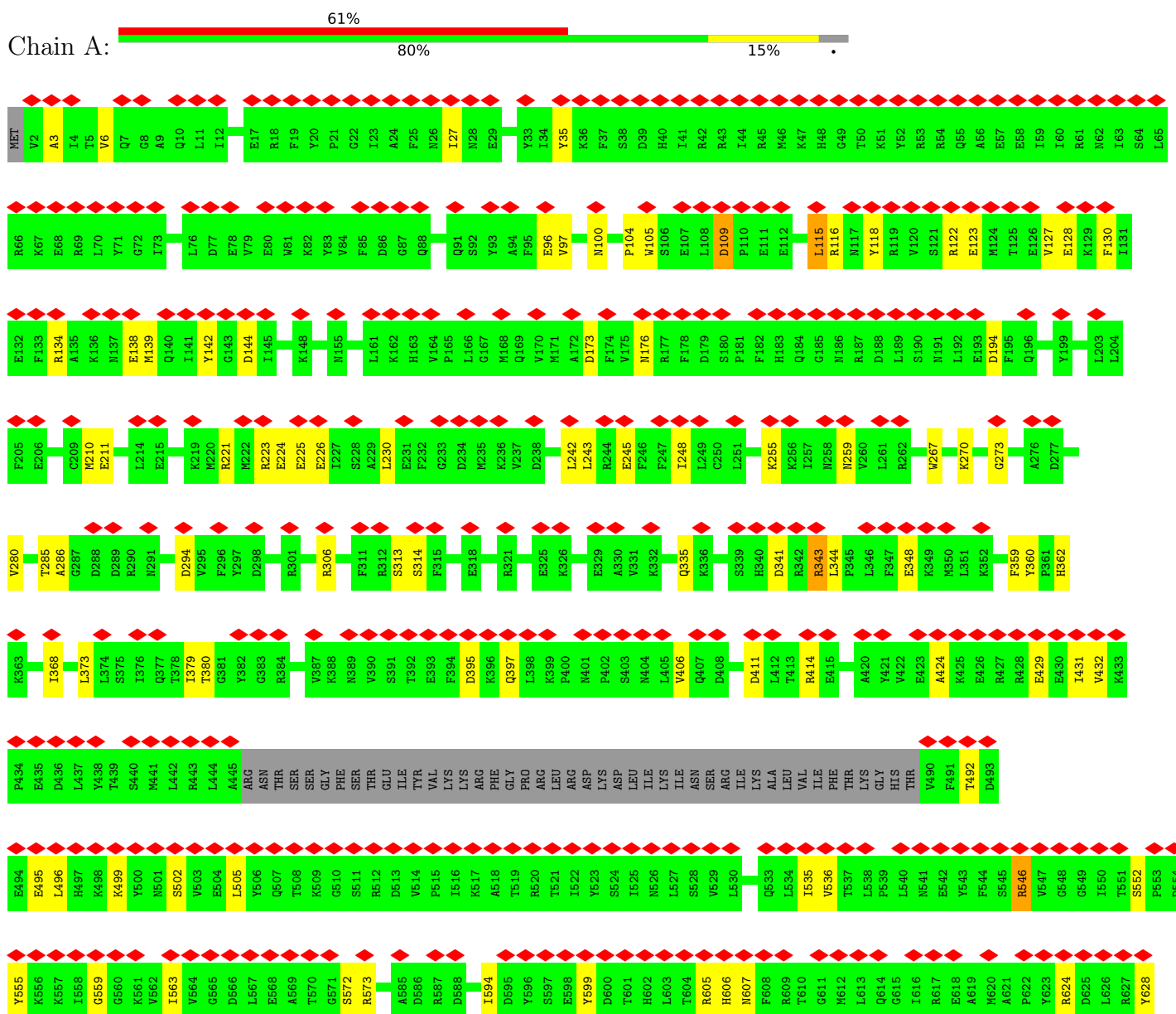
- Molecule 2 is a protein called Inner core structural protein VP3.

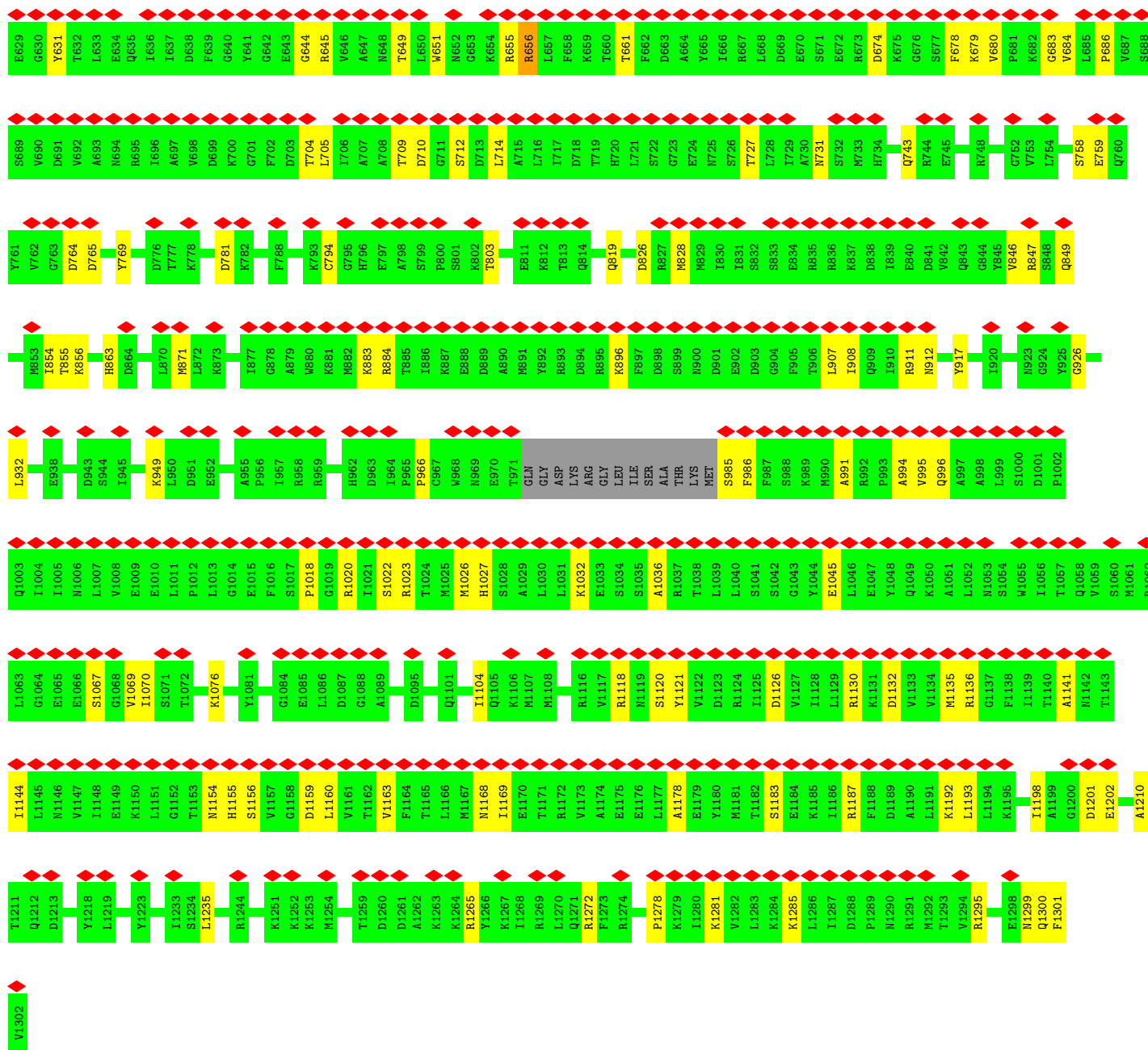
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	872	Total	C	N	O	S	0	0
			7046	4496	1222	1287	41		
2	C	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	D	863	Total	C	N	O	S	0	0
			6968	4448	1209	1271	40		
2	E	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	F	868	Total	C	N	O	S	0	0
			6995	4463	1209	1283	40		
2	G	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	H	868	Total	C	N	O	S	0	0
			7017	4476	1218	1282	41		
2	I	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	J	870	Total	C	N	O	S	0	0
			7030	4484	1220	1285	41		
2	K	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		

3 Residue-property plots

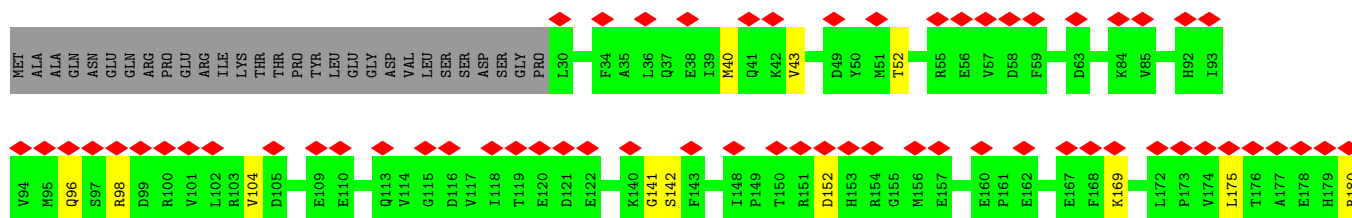
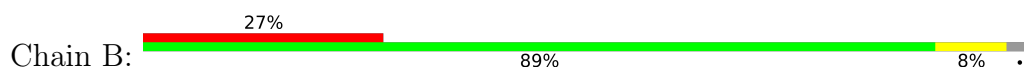
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

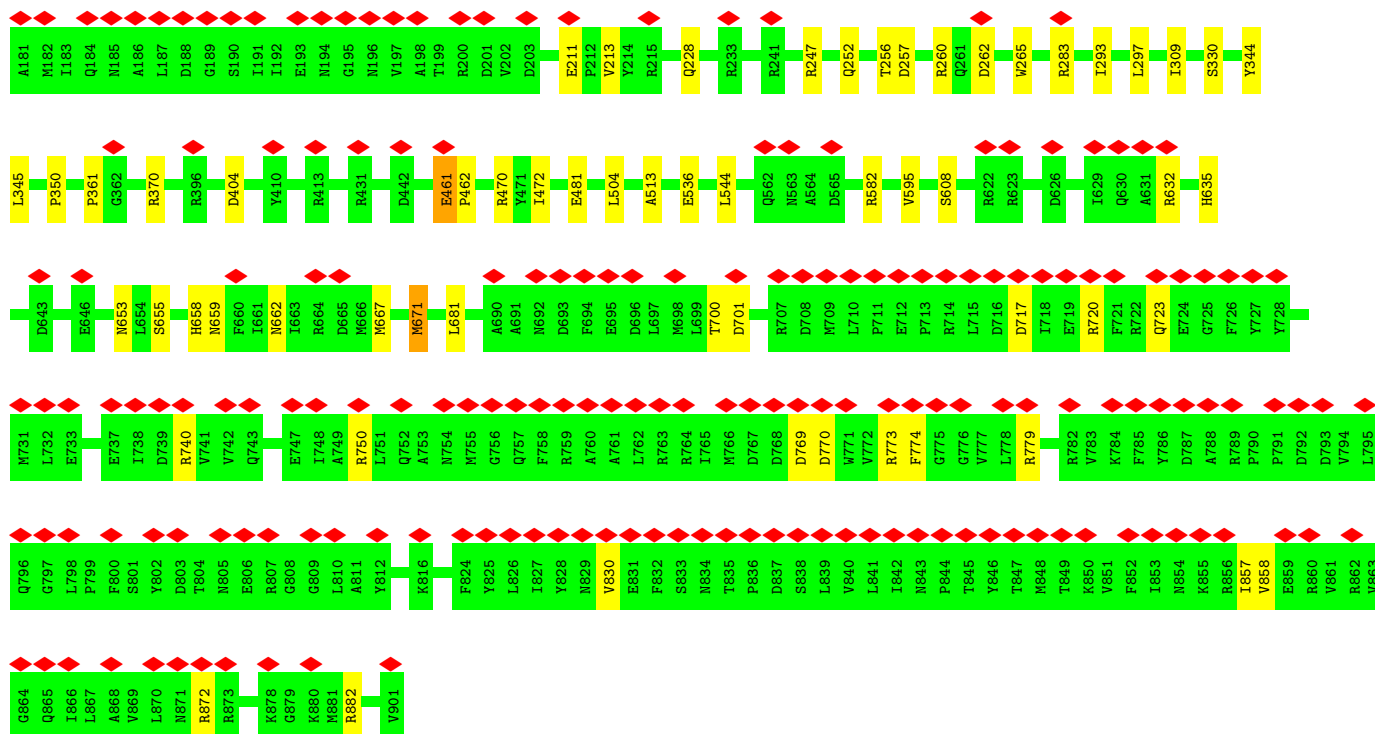
• Molecule 1: RNA-directed RNA polymerase



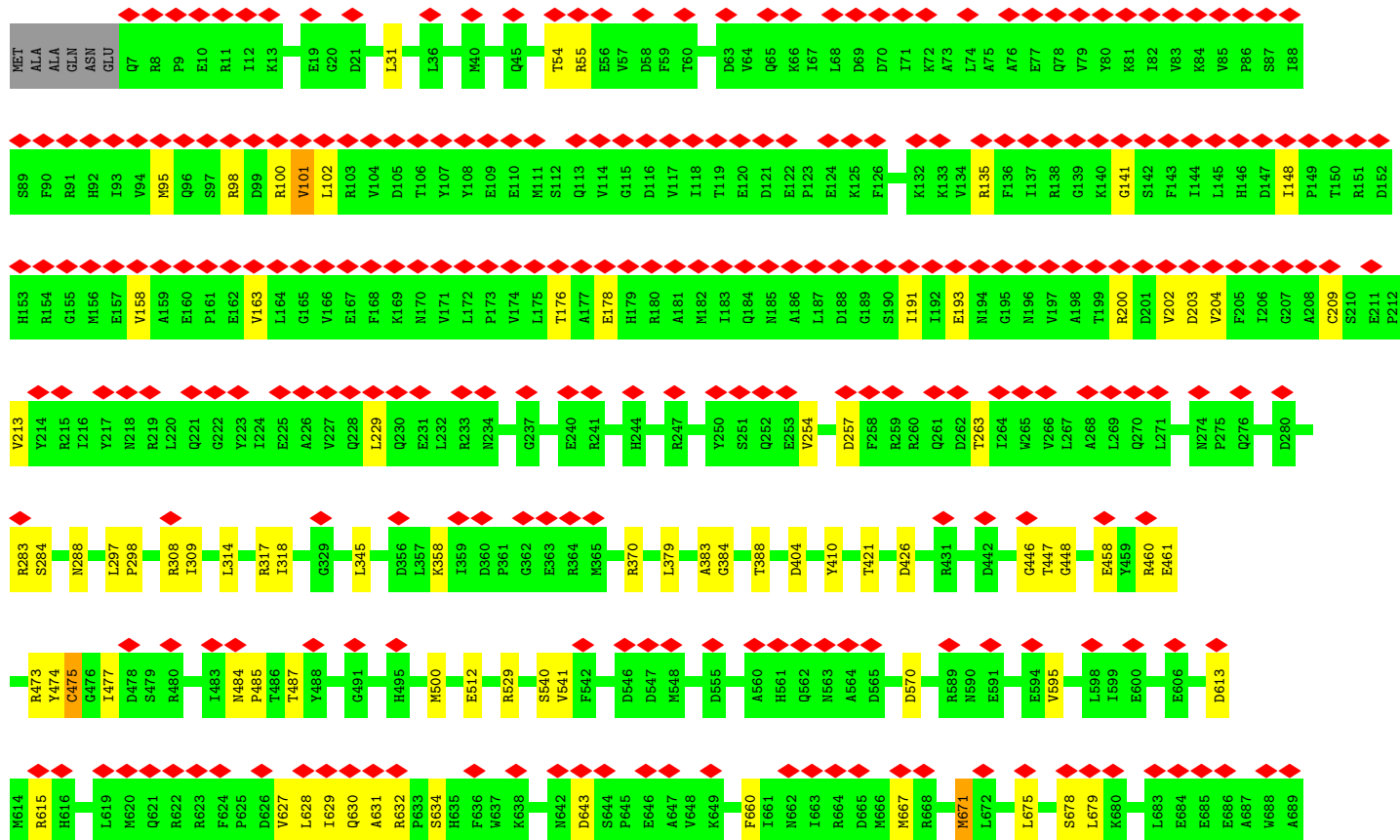
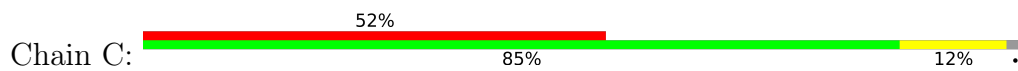


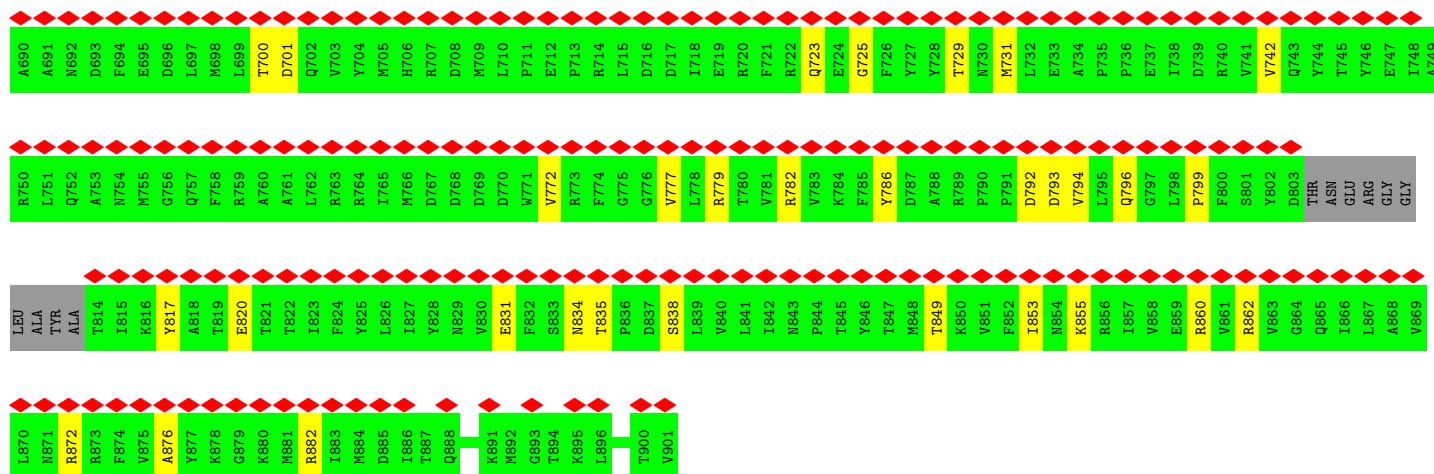
• Molecule 2: Inner core structural protein VP3



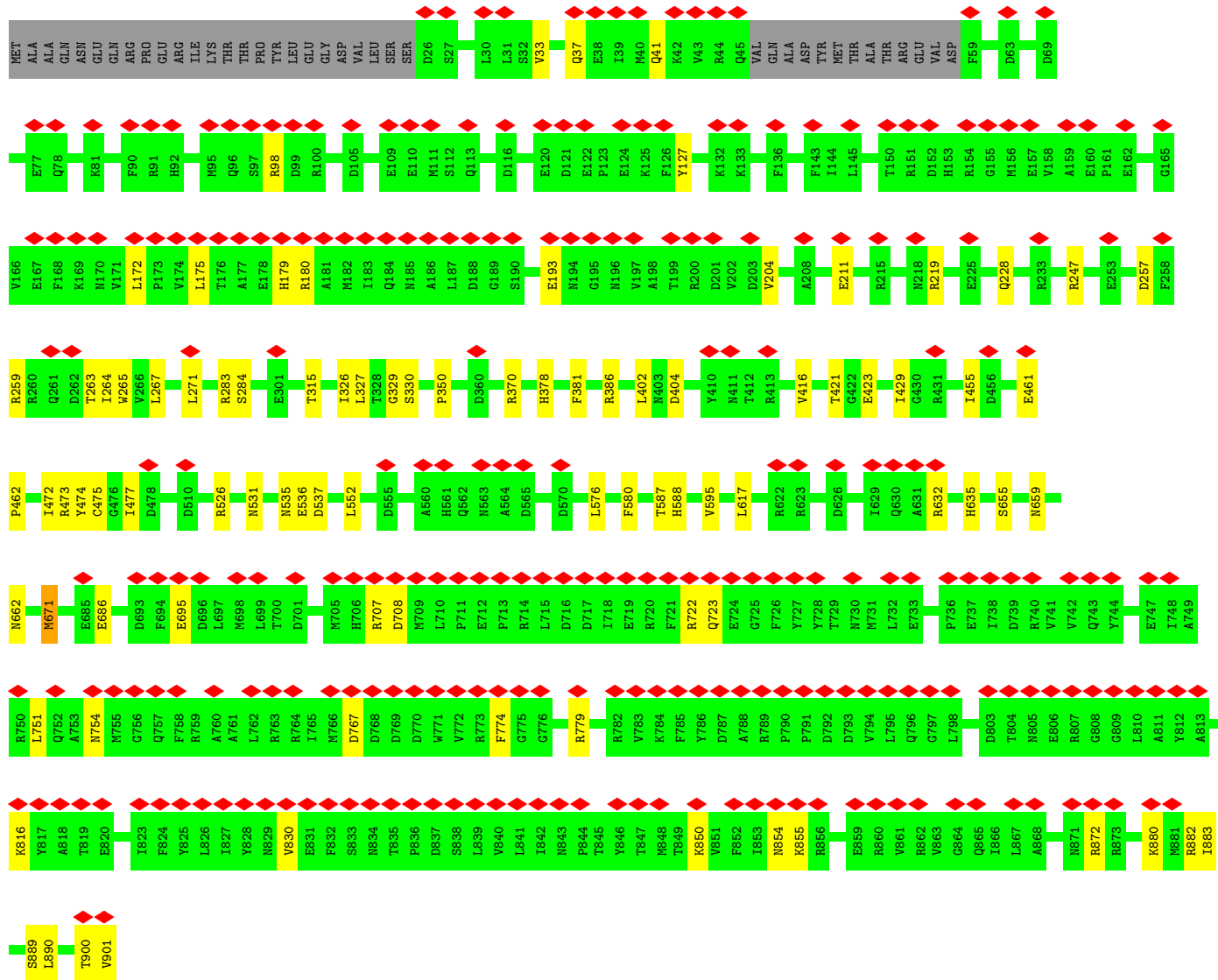
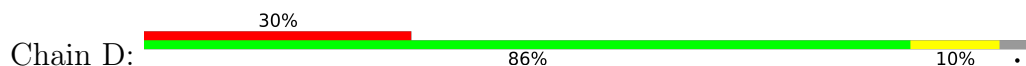


• Molecule 2: Inner core structural protein VP3



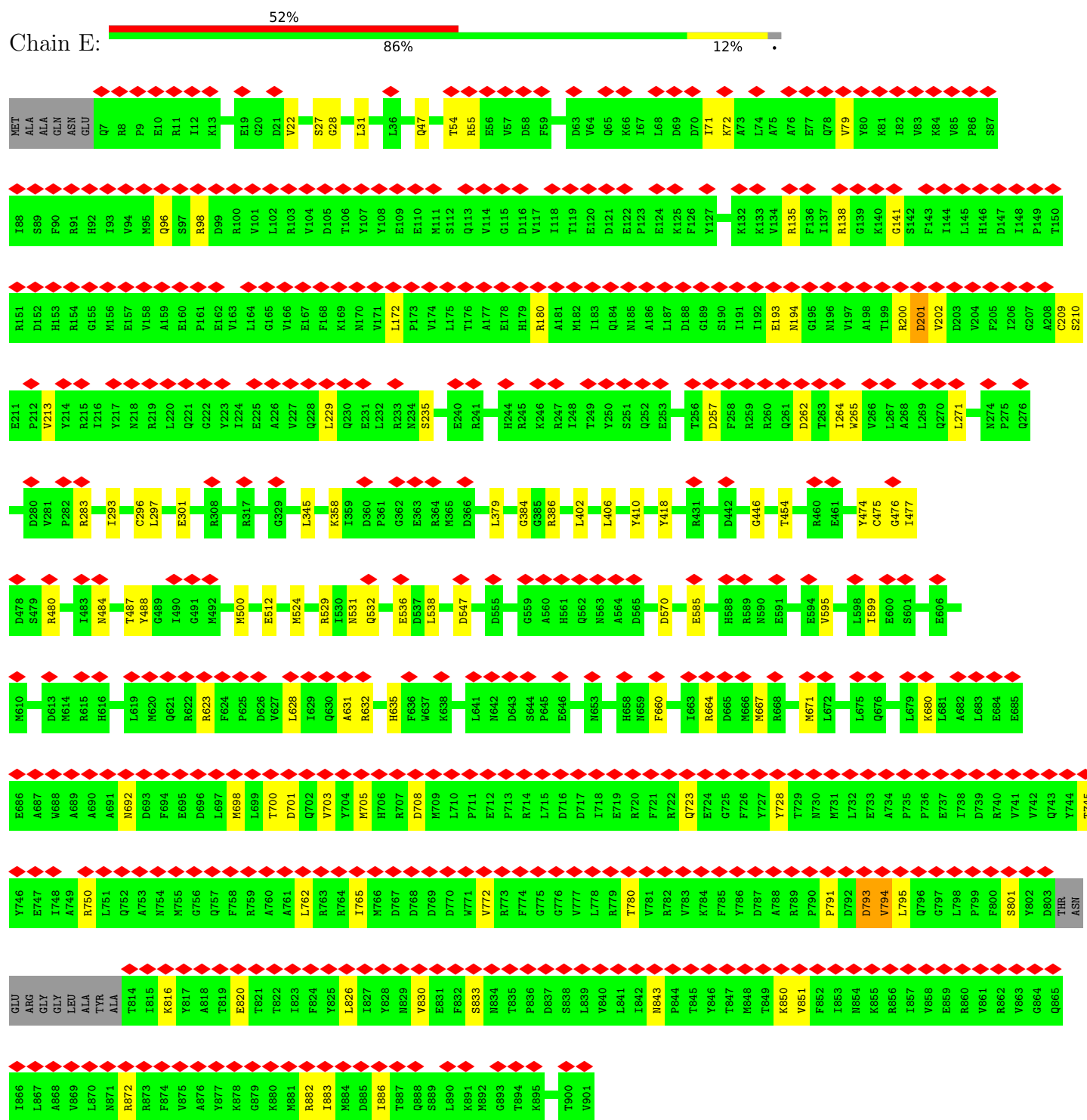


• Molecule 2: Inner core structural protein VP3



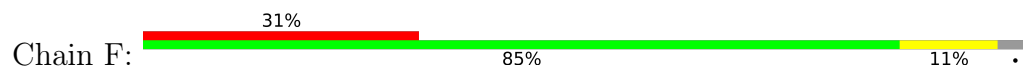
• Molecule 2: Inner core structural protein VP3

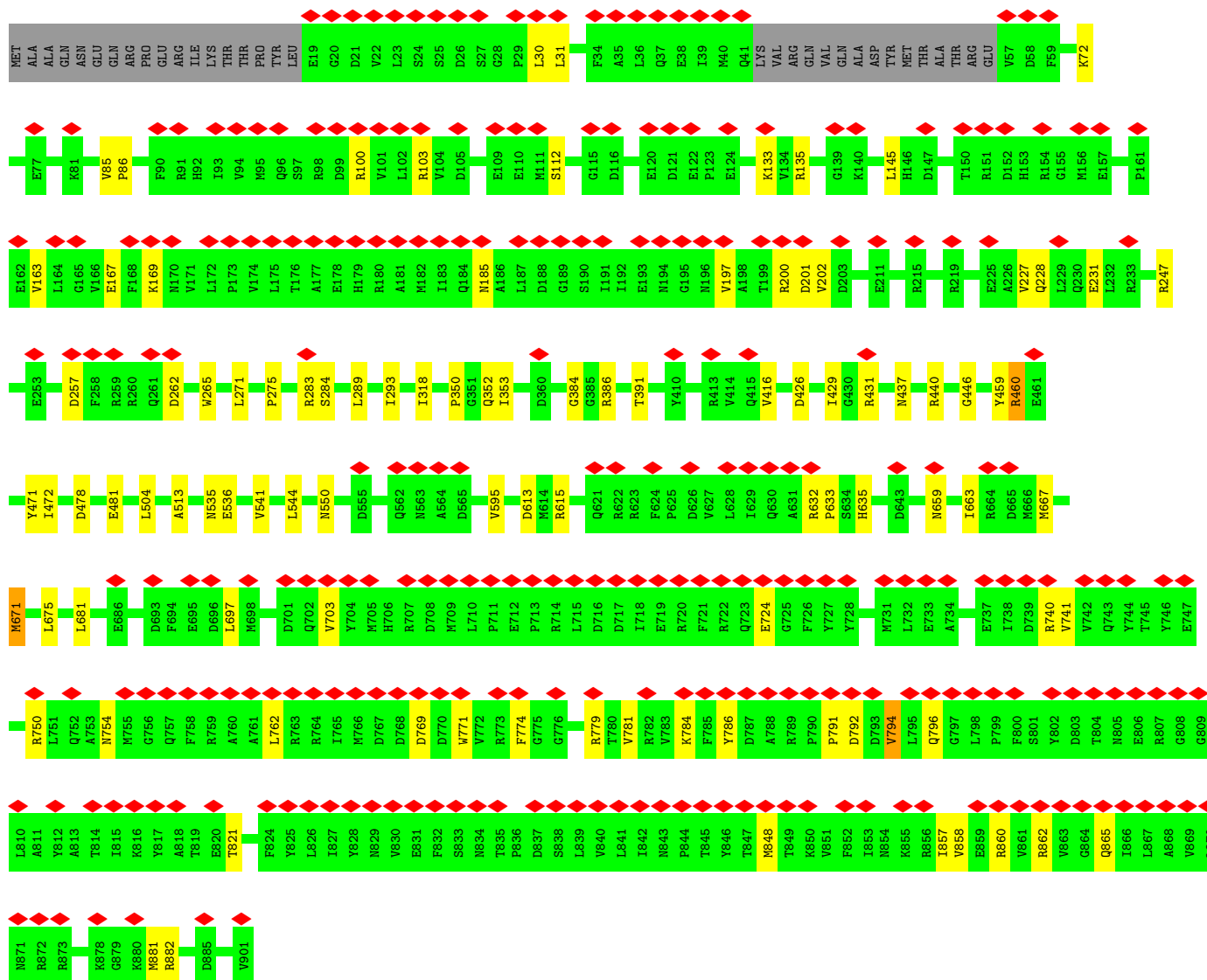
Chain E:



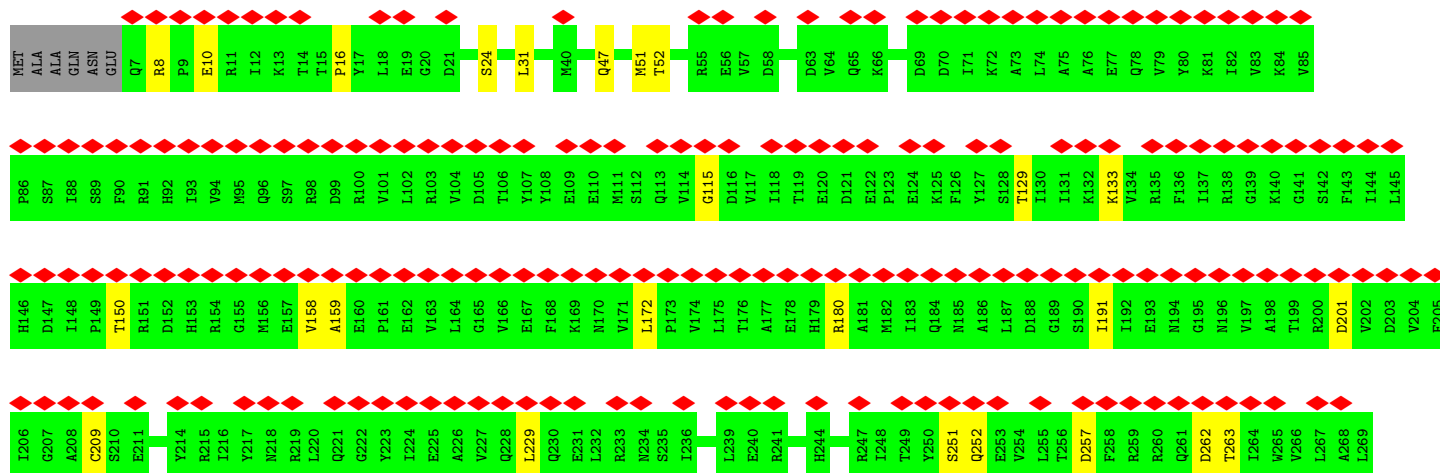
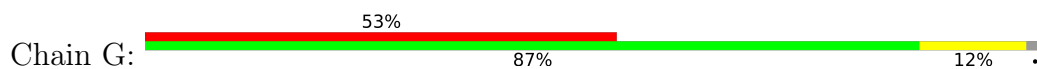
• Molecule 2: Inner core structural protein VP3

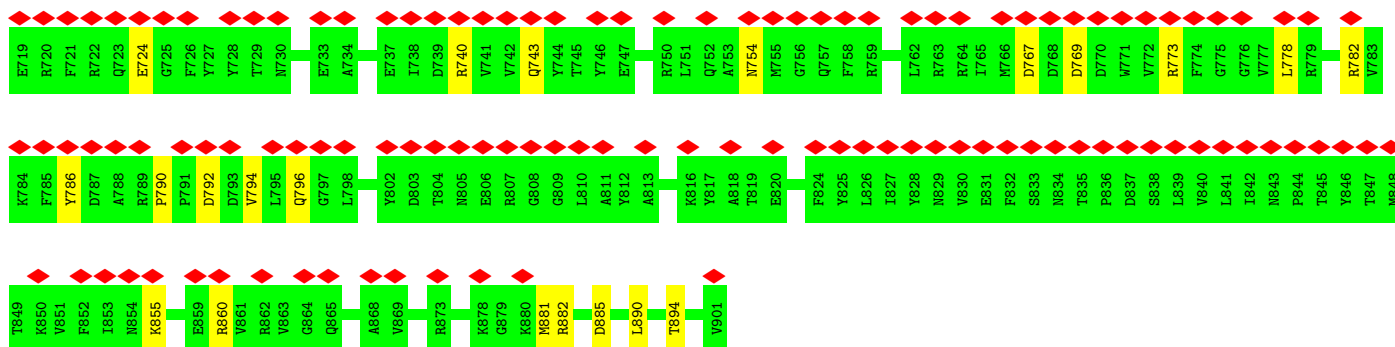
Chain F:



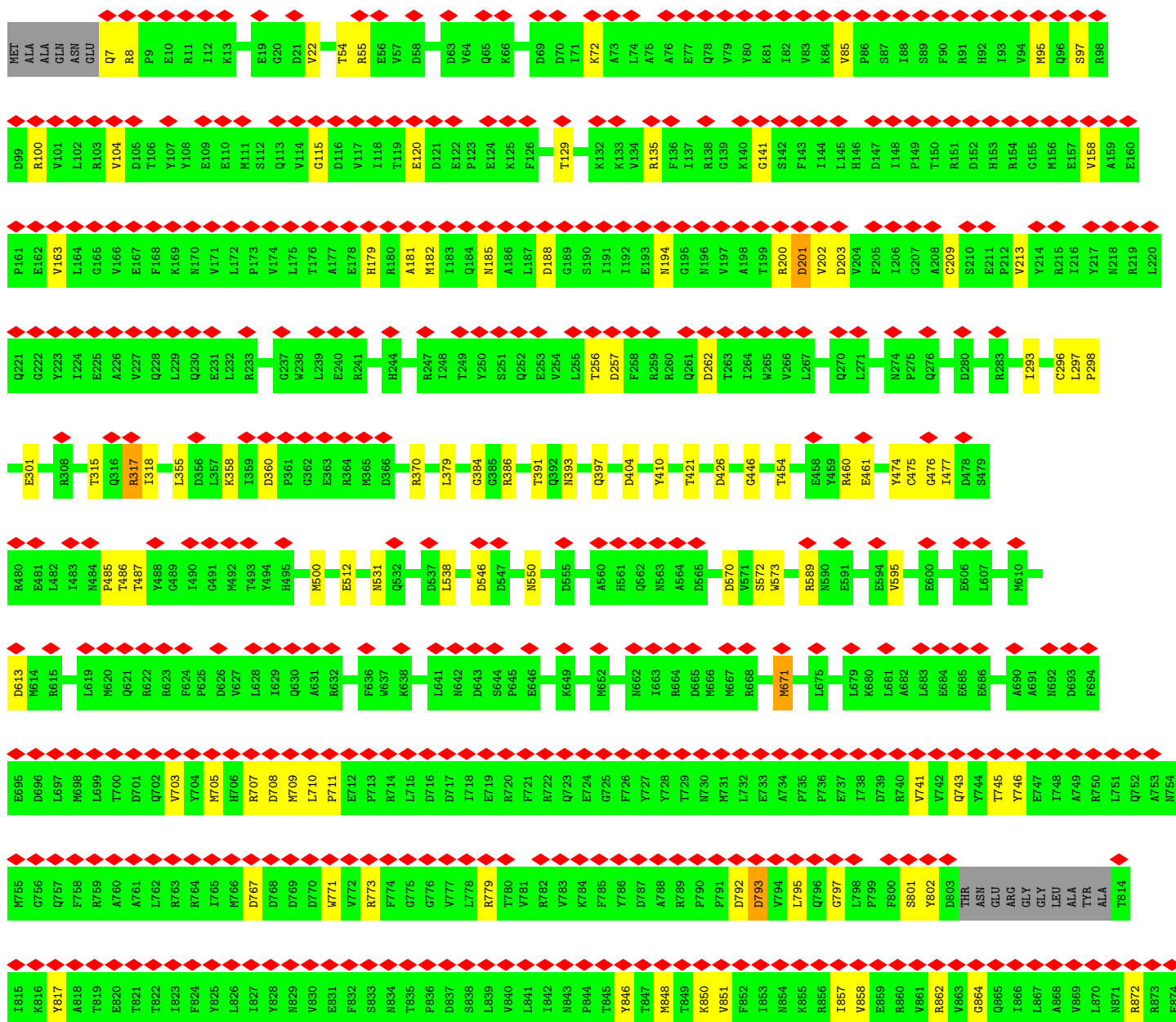
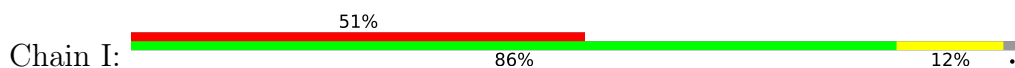


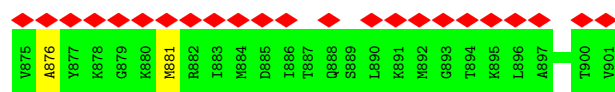
• Molecule 2: Inner core structural protein VP3



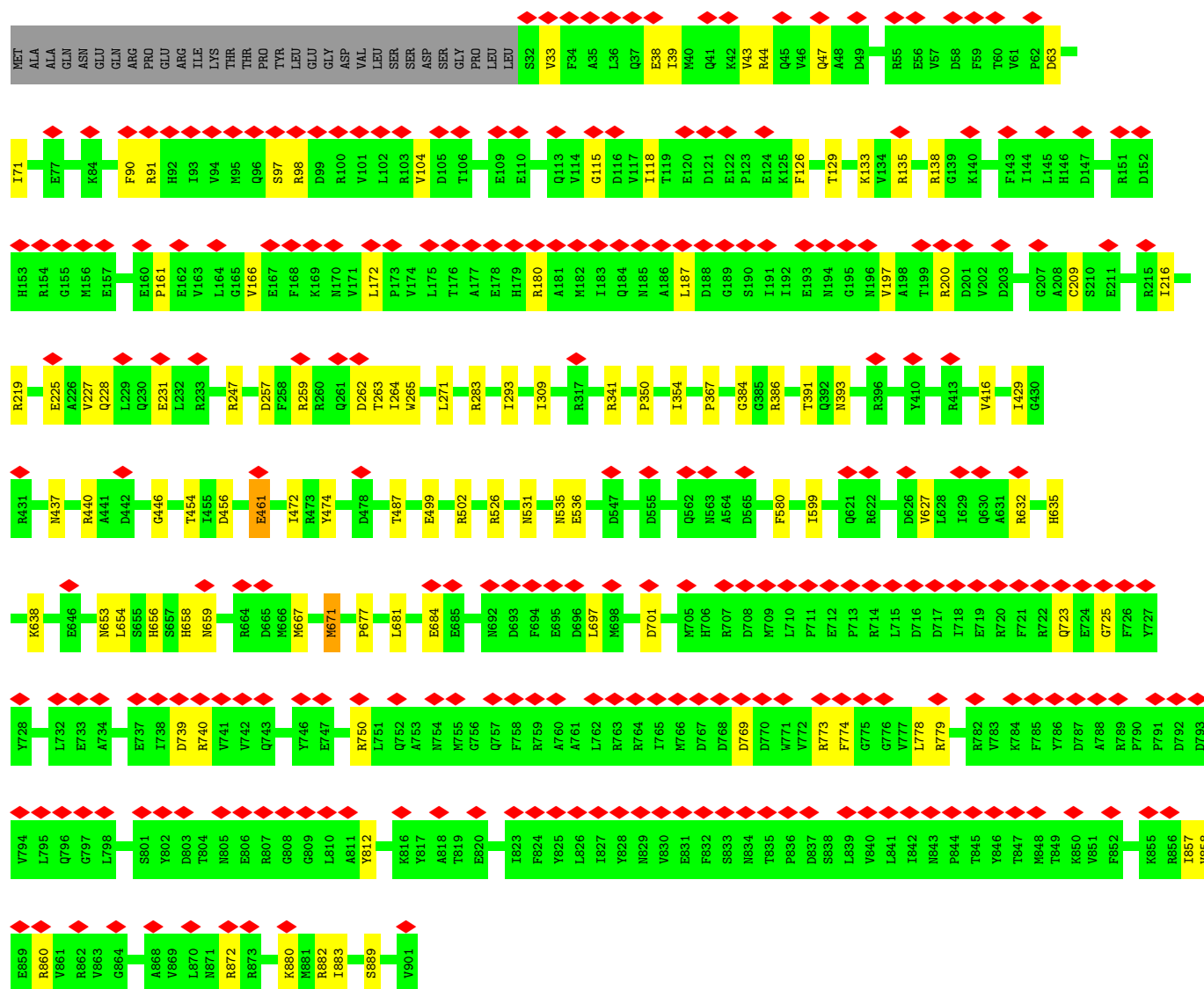
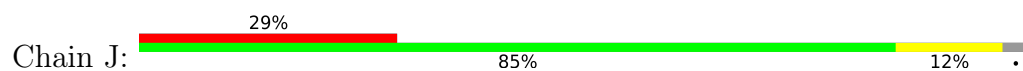


• Molecule 2: Inner core structural protein VP3

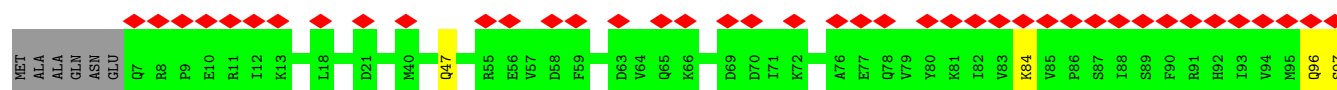
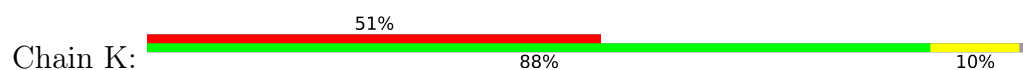




• Molecule 2: Inner core structural protein VP3



• Molecule 2: Inner core structural protein VP3



R873	R874	V875	A876	K878	G879	K880	M881	R882	I883	N884	D885	I886	T887	S888	S889	L890	K891	K895	A898	P899	T900	Y901																																						
ALA	T814	I815	V875	K816	Y817	R818	T819	E820	T821	T822	I823	F824	Y825	L826	I827	Y828	N829	V830	E831	F832	S833	N834	T835	P836	D837	S838	L839	V840	L841	I842	N843	P844	T845	Y846	T847	M848	T849	K850	V851	F852	I853	N854	K855	R856	I857	V858	E859	R860	V861	R862	V863	G864	Q865	I866	L867	A868	V869	L870	N871	R872
A753	M754	M755	G756	Q757	F758	R759	A760	A761	L762	R763	R764	I765	M766	D767	D768	D769	D770	Y771	V772	R773	F774	G775	G776	V777	L778	R779	T780	V781	R782	V783	K784	F785	Y786	D787	A788	R789	P790	P791	D792	D793	V794	L795	Q796	G797	L798	P799	F900	S901	Y902	D903	THR	ASN	GLU	ARG	GLY	GLY	LEU	ALA	TTR	
D693	F694	E695	D696	L697	M698	L699	T700	D701	Q702	V703	Y704	M705	H706	R707	D708	M709	L710	P711	E712	P713	R714	L715	D716	D717	I718	E719	R720	F721	R722	Q723	E724	G725	F726	Y727	Y728	I729	N730	M731	L732	E733	A734	P735	P736	E737	I738	D739	R740	V741	V742	Q743	Y744	T745	Y746	E747	I748	A749	R750	L751	Q752	
D613	M614	R615	H616	L619	M620	Q621	R622	R623	F624	P625	D626	V627	L628	I629	Q630	A631	R632	H635	K638	N642	D643	S644	P645	E646	K649	F660	I661	N662	L663	R664	D665	M666	M667	R668	M671	L672	L675	L679	K680	L681	A682	L683	E684	E685	E686	A689	A690	A691	N692											
D456	V457	R460	R470	R473	Y474	C475	A476	I477	R480	E481	L482	I483	M484	I490	M500	D510	M524	N531	L544	P545	D546	D547	L552	D555	A560	H561	Q562	N563	A564	D565	D570	H588	R589	N590	E591	L598	I599	E600	E606	K611	V612																			
T315	Q316	R317	A325	G329	T333	Q336	I354	K358	T359	D360	P361	G362	E363	R364	M365	R370	H378	L379	T382	A383	G384	G385	R386	T391	R396	L402	M403	D404	M411	Y418	R431	V438	D442	G446	T447	W452	A453	T454	I455																					
R219	L220	Q221	Q222	Y223	L224	E225	A226	V227	Q228	L229	Q230	E231	L232	R233	N234	E240	R241	H244	R247	I248	T249	Y250	S251	Q252	E253	V254	L255	T256	D257	F258	R259	R260	Q261	D262	T263	I264	W265	V266	L267	A268	L269	Q270	L271	N274	D280	R283	I293	L297	R308	I309										
A159	E160	P161	E162	V163	L164	G165	V166	E167	F168	K169	N170	V171	L172	P173	V174	L175	T176	A177	E178	H179	R180	A181	M182	I183	Q184	N185	A186	L187	D188	G189	S190	I191	I192	E193	N194	G195	N196	V197	A198	T199	R200	D201	V202	D203	V204	F205	I206	G207	A208	C209	S210	E211	P212	V213	V214	R215	I216	Y217	N218	
R98	D99	R100	V101	L102	R103	V104	D105	T106	Y107	Y108	E109	E110	M111	S112	Q113	V114	G115	D116	V117	I118	T119	E120	D121	E122	P123	E124	K125	F126	Y127	S128	T129	K132	K133	V134	R135	F136	I137	R138	G139	K140	G141	S142	F143	I144	L145	H146	D147	I148	P149	T150	R151	D152	H153	R154	G155	M156	E157	V158		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.0	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	0.076	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.31	0/10268	0.52	0/13862
2	B	0.36	0/7203	0.52	0/9782
2	C	0.33	0/7310	0.50	0/9927
2	D	0.37	0/7124	0.52	0/9673
2	E	0.32	0/7310	0.50	0/9927
2	F	0.37	0/7151	0.53	0/9712
2	G	0.33	0/7310	0.52	0/9927
2	H	0.37	0/7174	0.53	0/9742
2	I	0.33	0/7310	0.51	0/9927
2	J	0.37	0/7187	0.53	0/9760
2	K	0.33	0/7310	0.51	0/9927
All	All	0.34	0/82657	0.52	0/112166

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	10062	0	10106	128	0
2	B	7046	0	7032	56	0
2	C	7151	0	7137	74	0
2	D	6968	0	6955	68	0
2	E	7151	0	7137	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	6995	0	6968	68	0
2	G	7151	0	7137	69	0
2	H	7017	0	6996	77	0
2	I	7151	0	7137	74	0
2	J	7030	0	7010	73	0
2	K	7151	0	7137	77	0
All	All	80873	0	80752	770	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 5.

The worst 5 of 770 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:K:438:VAL:HG11	2:K:452:TRP:CZ2	1.57	1.37
2:K:438:VAL:HG11	2:K:452:TRP:CH2	1.65	1.32
2:D:461:GLU:CG	2:D:462:PRO:HD3	1.67	1.23
2:K:438:VAL:CG1	2:K:452:TRP:CZ2	2.23	1.21
2:G:595:VAL:HG22	2:G:891:LYS:NZ	1.60	1.16

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	1238/1302 (95%)	1153 (93%)	85 (7%)	0	100	100
2	B	870/901 (97%)	829 (95%)	41 (5%)	0	100	100
2	C	881/901 (98%)	825 (94%)	56 (6%)	0	100	100
2	D	859/901 (95%)	828 (96%)	31 (4%)	0	100	100
2	E	881/901 (98%)	828 (94%)	53 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	864/901 (96%)	822 (95%)	42 (5%)	0	100	100
2	G	881/901 (98%)	836 (95%)	45 (5%)	0	100	100
2	H	866/901 (96%)	813 (94%)	53 (6%)	0	100	100
2	I	881/901 (98%)	829 (94%)	52 (6%)	0	100	100
2	J	868/901 (96%)	821 (95%)	47 (5%)	0	100	100
2	K	881/901 (98%)	830 (94%)	51 (6%)	0	100	100
All	All	9970/10312 (97%)	9414 (94%)	556 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	1110/1161 (96%)	1099 (99%)	11 (1%)	76	88
2	B	767/792 (97%)	765 (100%)	2 (0%)	92	97
2	C	782/792 (99%)	777 (99%)	5 (1%)	86	94
2	D	759/792 (96%)	755 (100%)	4 (0%)	88	95
2	E	782/792 (99%)	776 (99%)	6 (1%)	81	91
2	F	763/792 (96%)	755 (99%)	8 (1%)	76	88
2	G	782/792 (99%)	778 (100%)	4 (0%)	88	95
2	H	763/792 (96%)	761 (100%)	2 (0%)	92	97
2	I	782/792 (99%)	776 (99%)	6 (1%)	81	91
2	J	765/792 (97%)	761 (100%)	4 (0%)	88	95
2	K	782/792 (99%)	777 (99%)	5 (1%)	86	94
All	All	8837/9081 (97%)	8780 (99%)	57 (1%)	86	94

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	271	LEU
2	K	671	MET
2	F	794	VAL
2	K	570	ASP
2	J	461	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	417	ASN
2	K	433	GLN
2	I	653	ASN
2	J	535	ASN
2	D	433	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.

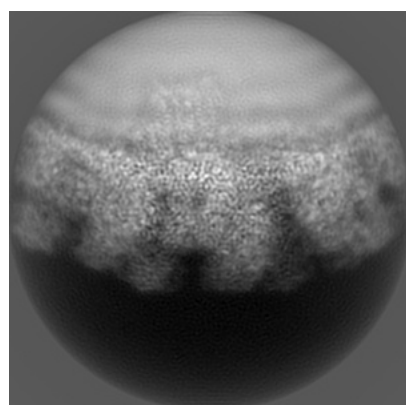
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20407. These allow visual inspection of the internal detail of the map and identification of artifacts.

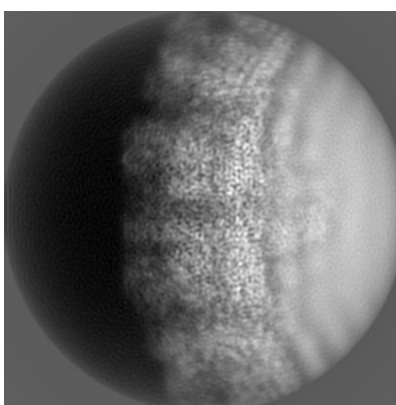
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

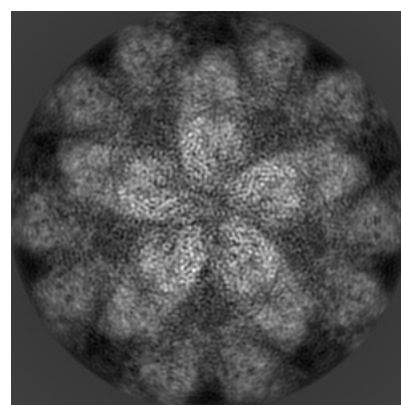
6.1.1 Primary map



X



Y

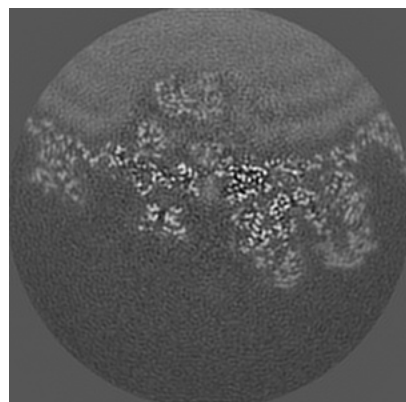


Z

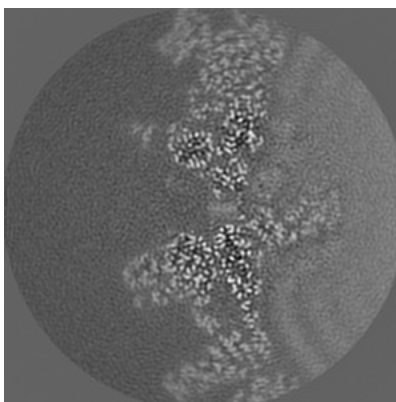
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

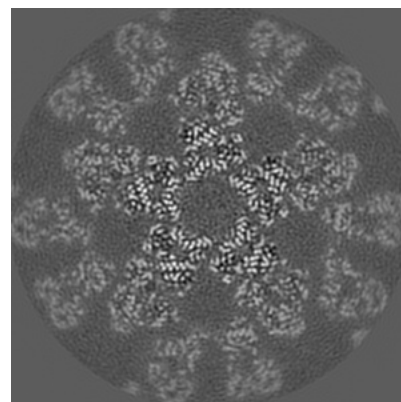
6.2.1 Primary map



X Index: 128



Y Index: 128

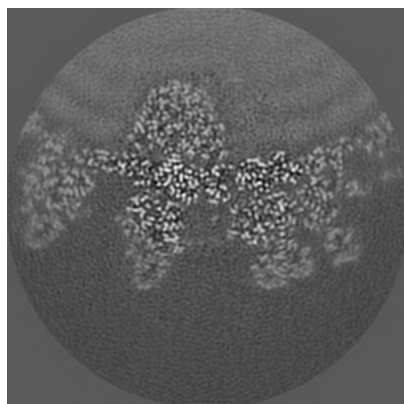


Z Index: 128

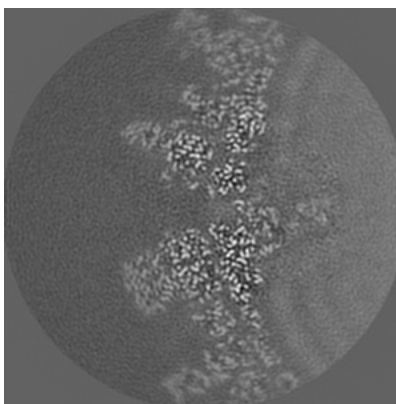
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

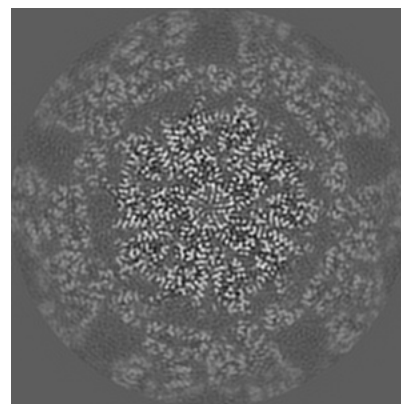
6.3.1 Primary map



X Index: 114



Y Index: 132



Z Index: 149

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

6.4 Orthogonal surface views [i](#)

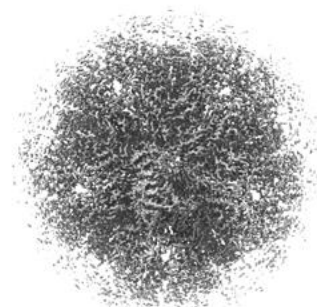
6.4.1 Primary map



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.

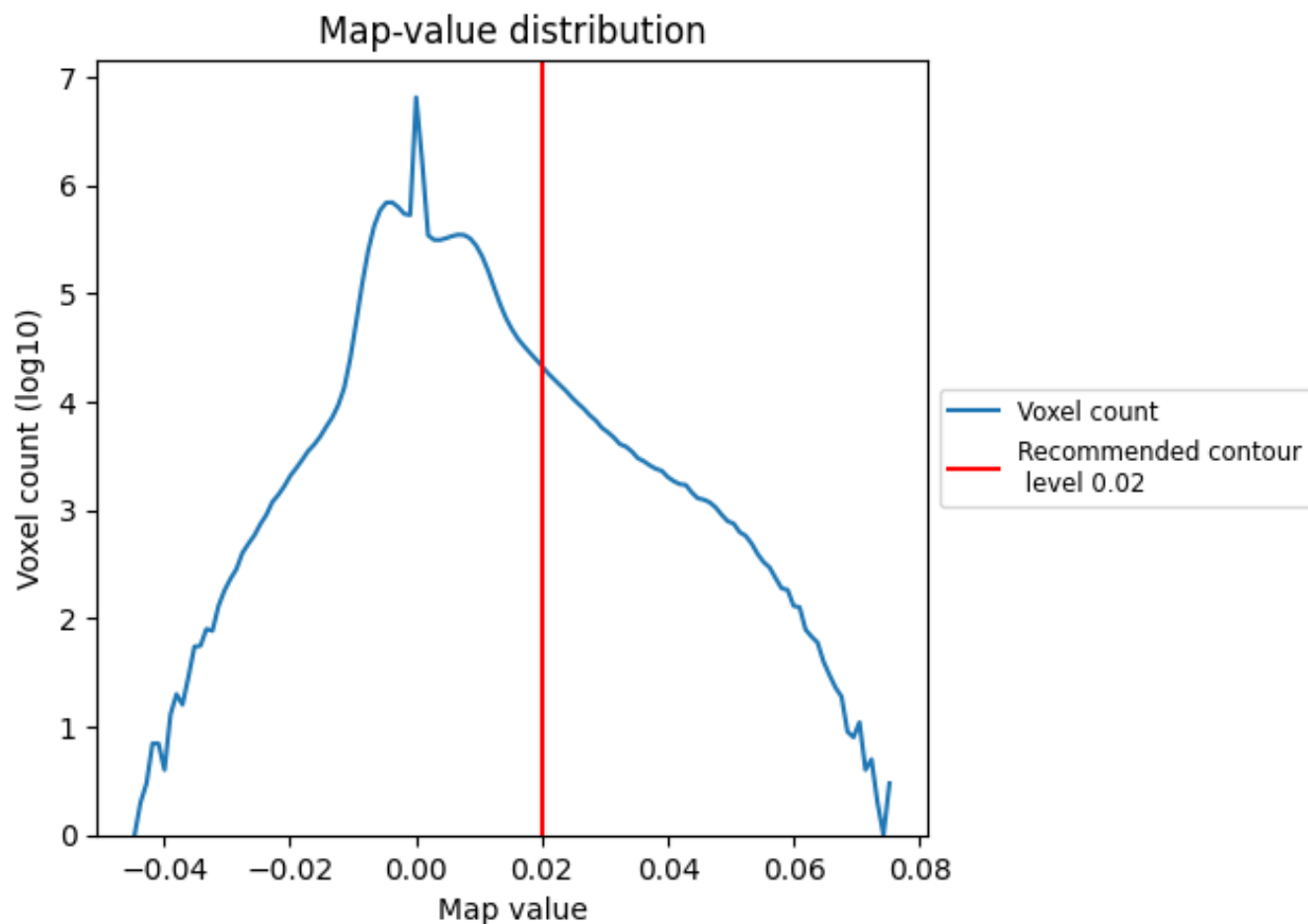
6.5 Mask visualisation

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

7 Map analysis [i](#)

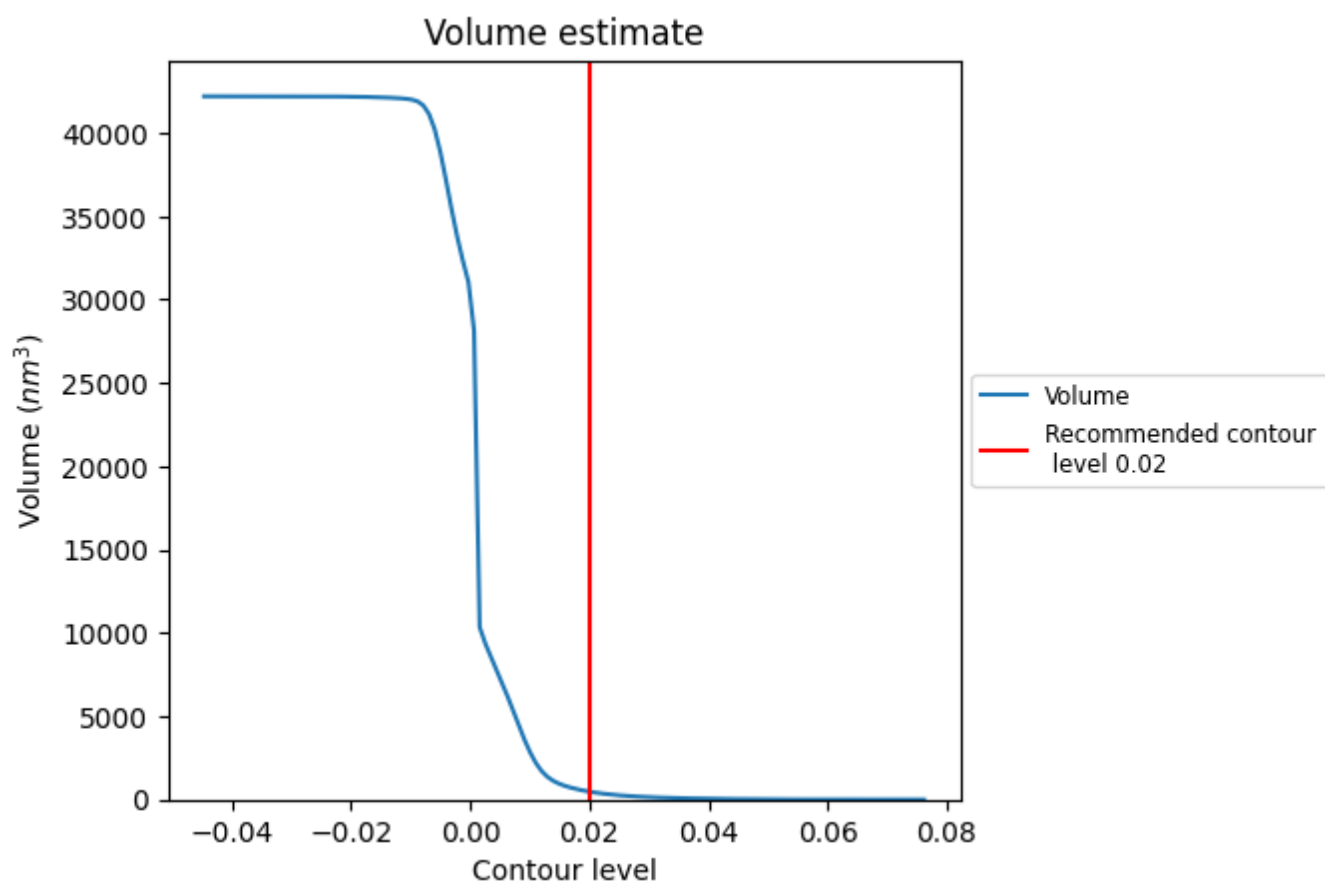
This section contains the results of statistical analysis of the map.

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.

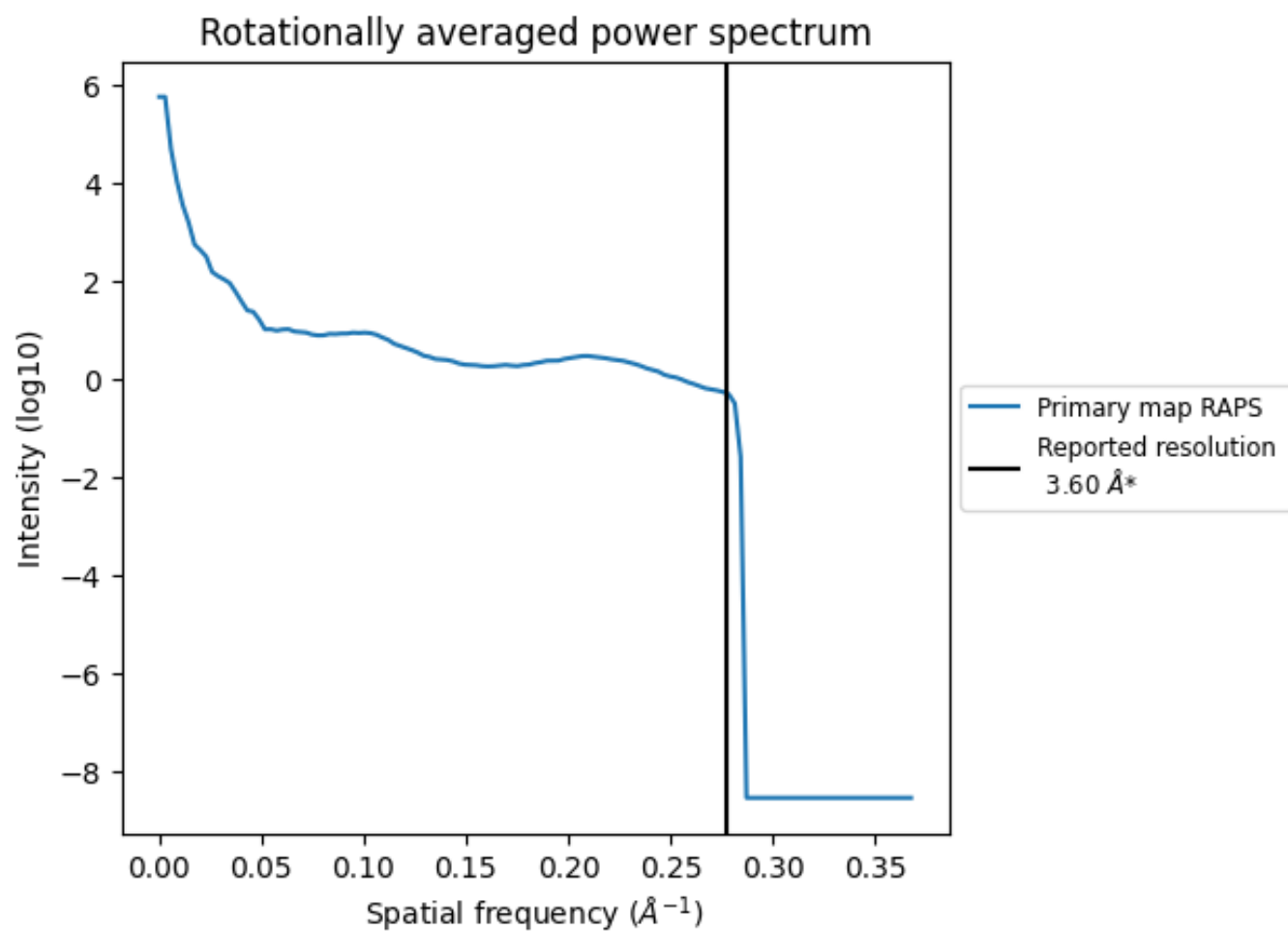
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 474 nm³; this corresponds to an approximate mass of 428 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 0.278 Å⁻¹

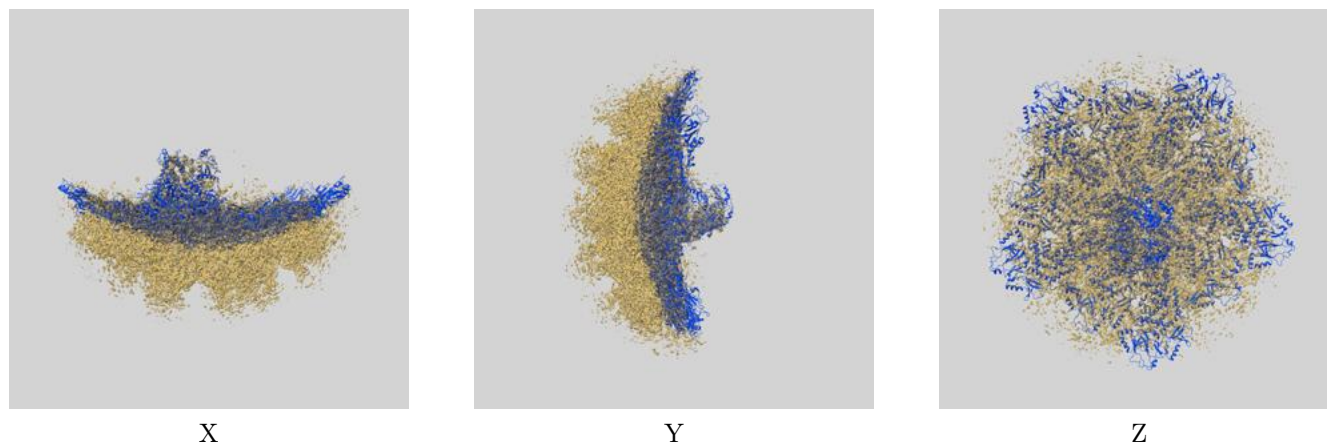
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

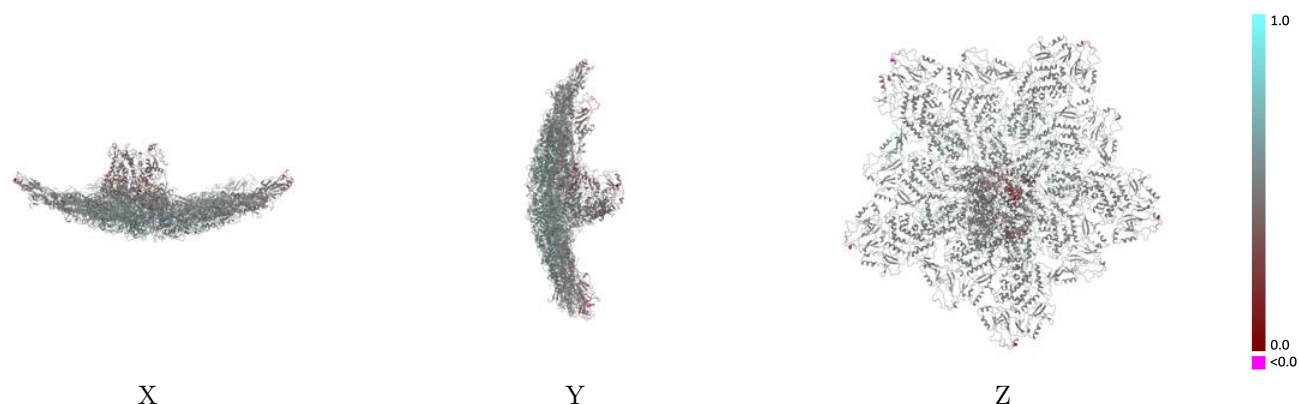
This section contains information regarding the fit between EMDB map EMD-20407 and PDB model 6PO2. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



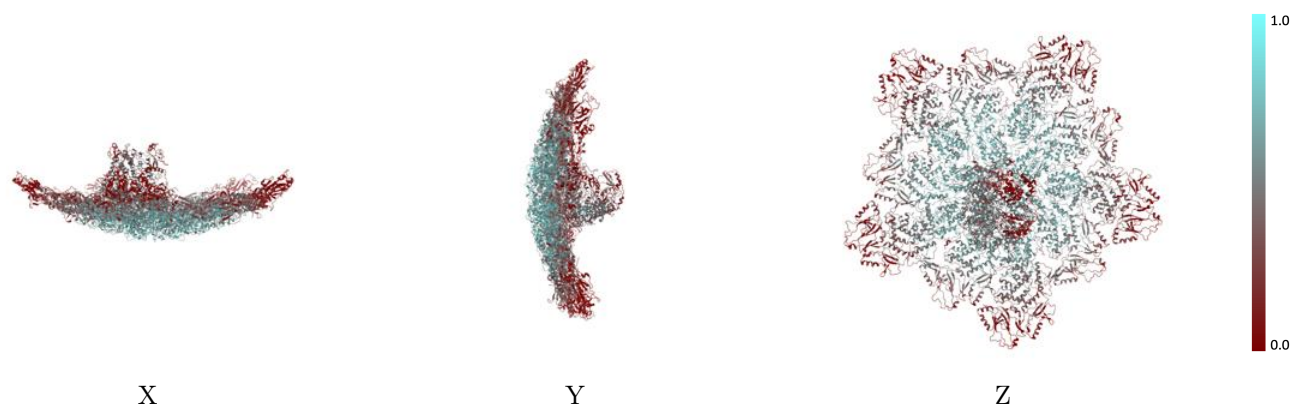
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



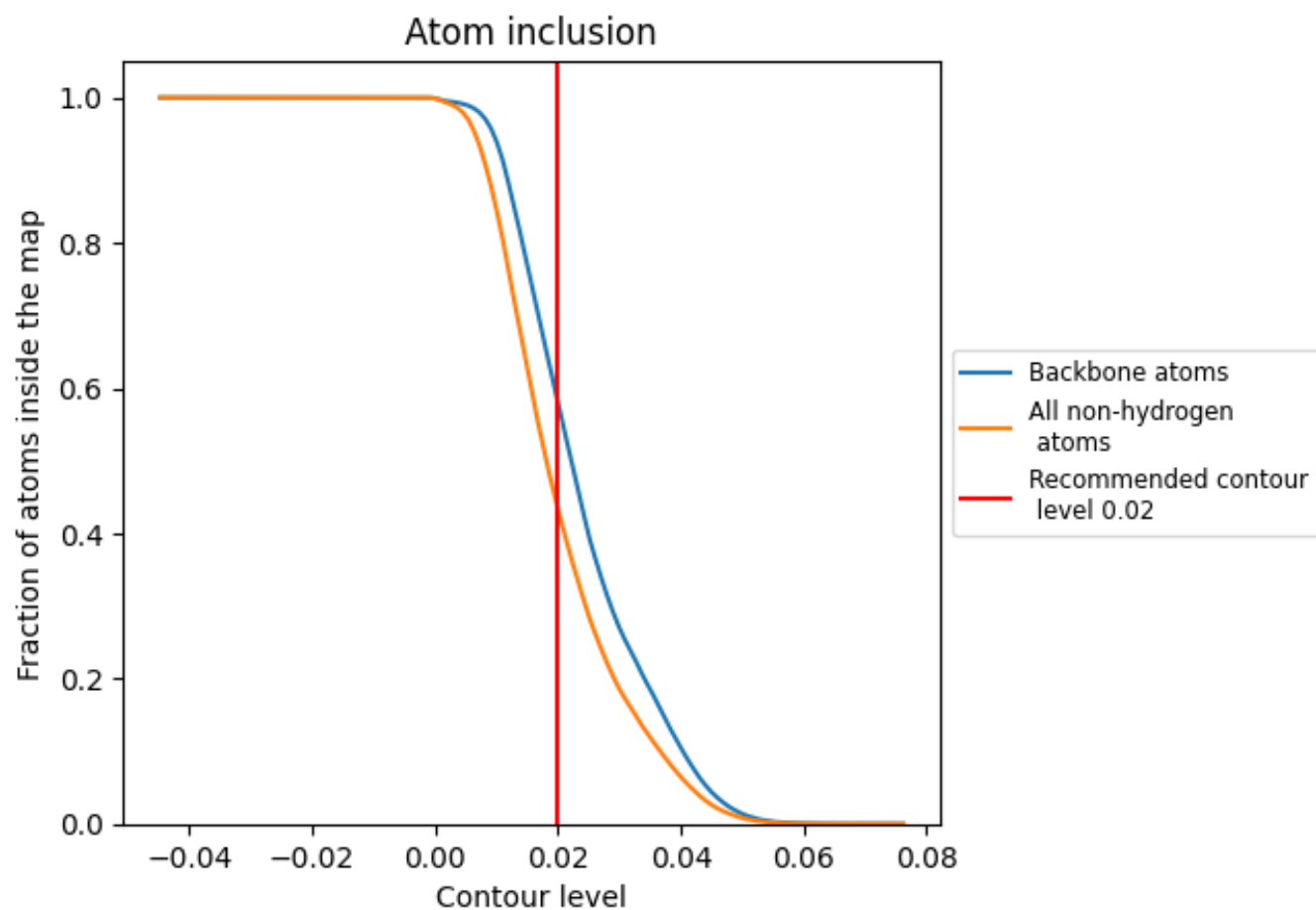
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4339	<div></div> 0.4970
A	<div></div> 0.3055	<div></div> 0.4370
B	<div></div> 0.5429	<div></div> 0.5230
C	<div></div> 0.3780	<div></div> 0.4900
D	<div></div> 0.5317	<div></div> 0.5200
E	<div></div> 0.3718	<div></div> 0.4890
F	<div></div> 0.5144	<div></div> 0.5160
G	<div></div> 0.3697	<div></div> 0.4880
H	<div></div> 0.5192	<div></div> 0.5150
I	<div></div> 0.3787	<div></div> 0.4930
J	<div></div> 0.5414	<div></div> 0.5240
K	<div></div> 0.3819	<div></div> 0.4920

1.0

0.0

<0.0