wwPDB EM Validation Summary Report

Oct 5, 2024 – 09:03 PM EDT

PDB ID	:	5VU2
EMDB ID	:	EMD-8734
Title	:	Electron cryo-microscopy of "immature" Chikungunya VLP
Authors	:	Rossmann, M.G.; Yap, M.L.
Deposited on	:	2017-05-18
Resolution	:	6.80 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:

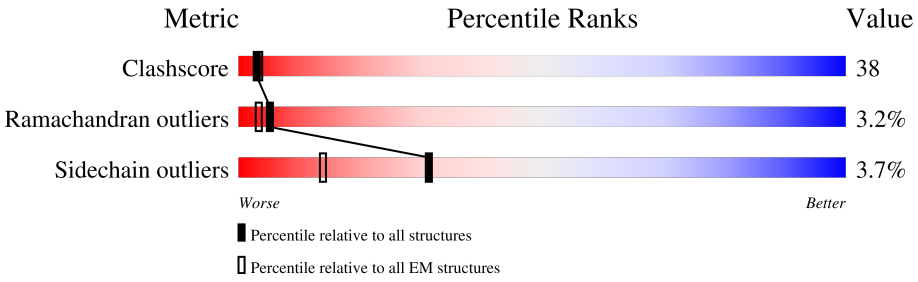
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 6.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	866	21% 37% · 61%
1	B	866	21% 36% · 61%
1	C	866	20% 36% · 61%
1	D	866	21% 36% · 61%
1	M	866	21% 41% · · 56%
1	N	866	25% 41% · 56%
1	O	866	20% 39% 5% 56%
1	P	866	19% 40% · 56%

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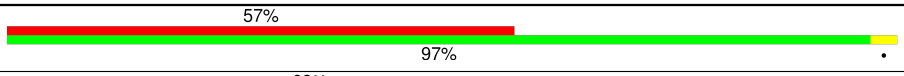
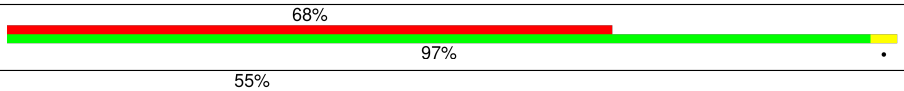
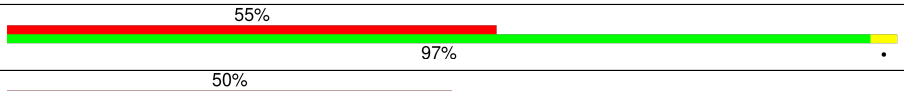
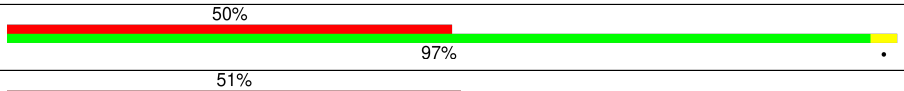
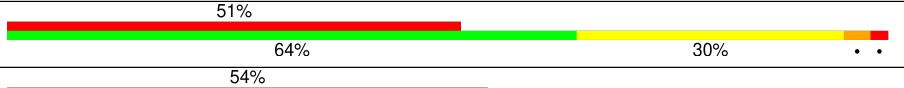
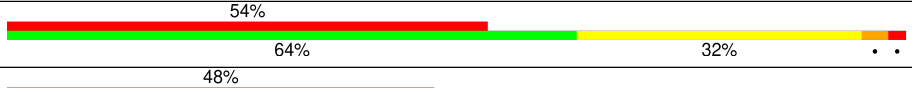
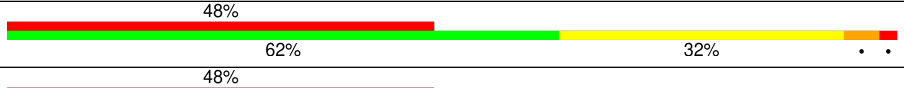
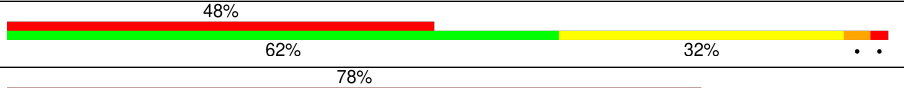
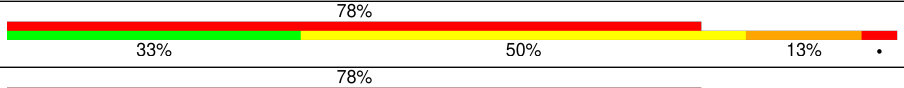
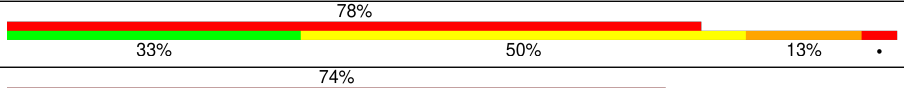
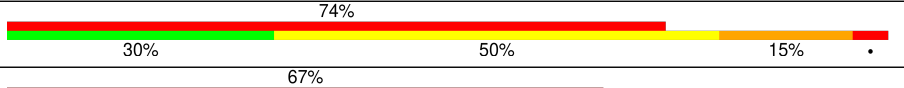
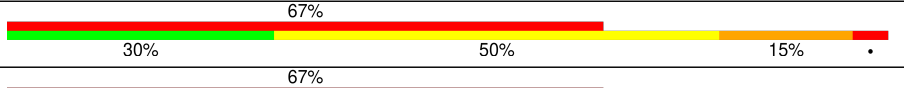
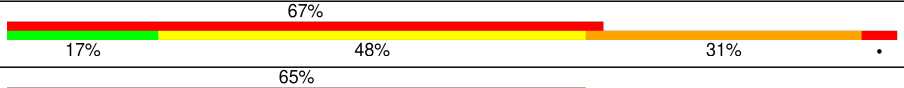
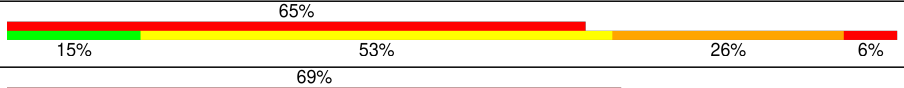
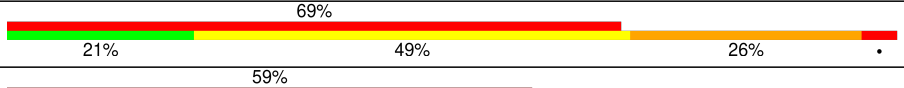
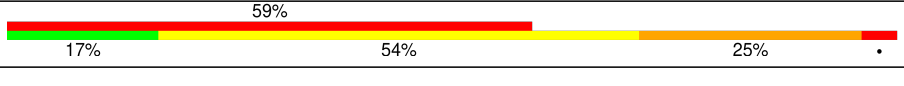
Mol	Chain	Length	Quality of chain
2	U	60	
2	V	60	
2	W	60	
2	X	60	
3	I	149	
3	J	149	
3	K	149	
3	L	149	
4	E	46	
4	F	46	
4	G	46	
4	H	46	
5	Q	81	
5	R	81	
5	S	81	
5	T	81	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32676 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 E1 envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		
1	A	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	B	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	N	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		
1	C	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	O	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		
1	D	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	P	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		

- Molecule 2 is a protein called E3 envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	60	Total	C	N	O	S	0	0
			477	296	81	91	9		
2	V	60	Total	C	N	O	S	0	0
			477	296	81	91	9		
2	W	60	Total	C	N	O	S	0	0
			477	296	81	91	9		
2	X	60	Total	C	N	O	S	0	0
			477	296	81	91	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	64	GLU	-	expression tag	UNP C7S7A1
V	64	GLU	-	expression tag	UNP C7S7A1

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Chain	Residue	Modelled	Actual	Comment	Reference
W	64	GLU	-	expression tag	UNP C7S7A1
X	64	GLU	-	expression tag	UNP C7S7A1

- Molecule 3 is a protein called capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		
3	J	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		
3	K	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		
3	L	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		

- Molecule 4 is a protein called E1 envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	46	Total	C	N	O	S	0	0
			336	218	57	59	2		
4	F	46	Total	C	N	O	S	0	0
			336	218	57	59	2		
4	G	46	Total	C	N	O	S	0	0
			336	218	57	59	2		
4	H	46	Total	C	N	O	S	0	0
			336	218	57	59	2		

- Molecule 5 is a protein called E2 envelope glycoprotein.

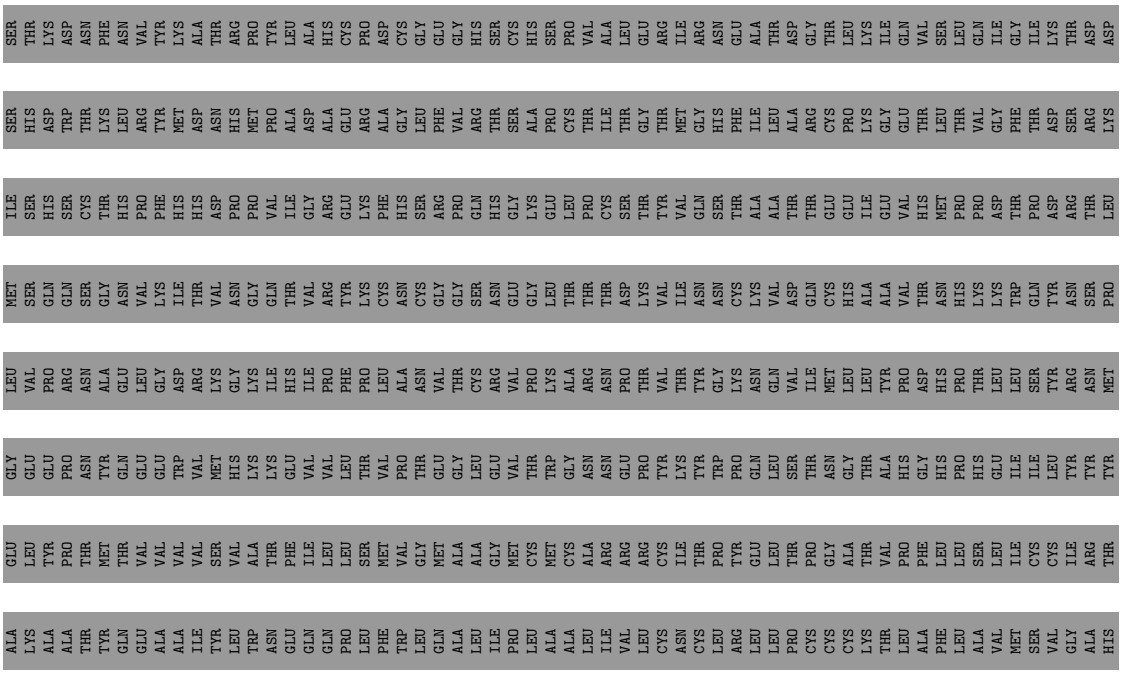
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	81	Total	C	N	O	S	0	0
			613	396	101	108	8		
5	R	81	Total	C	N	O	S	0	0
			613	396	101	108	8		
5	S	81	Total	C	N	O	S	0	0
			613	396	101	108	8		
5	T	81	Total	C	N	O	S	0	0
			613	396	101	108	8		

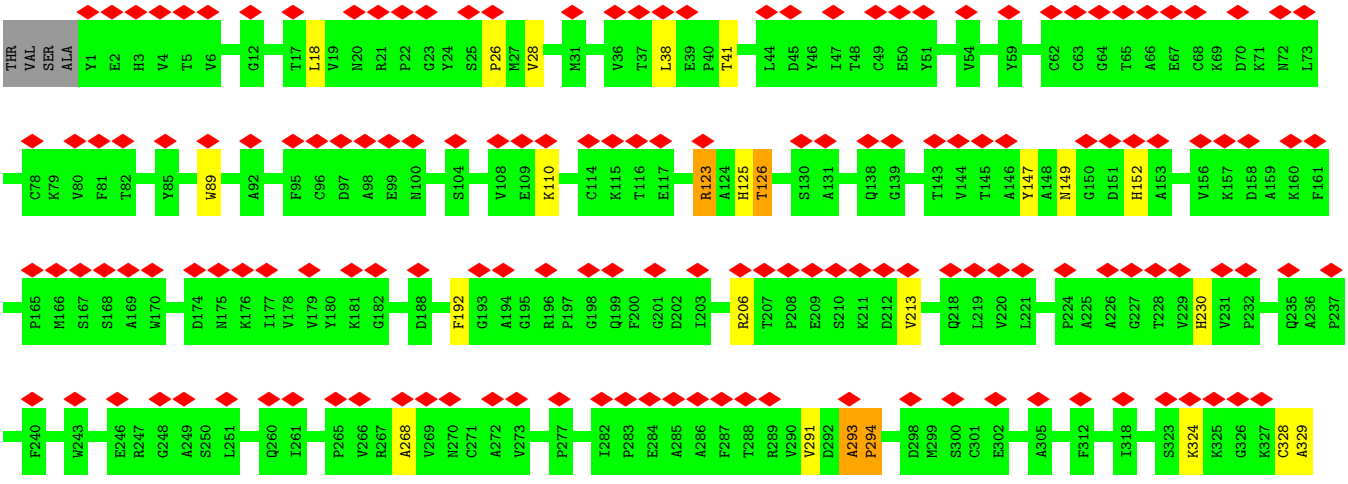
3 Residue-property plots (i)

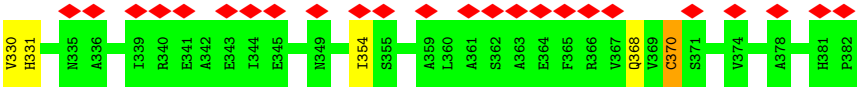
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E1 envelope glycoprotein

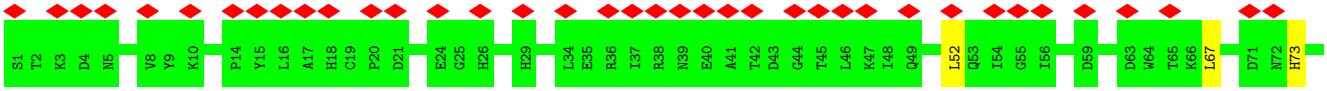
Chain M:

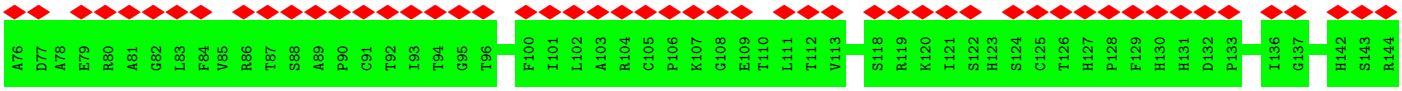


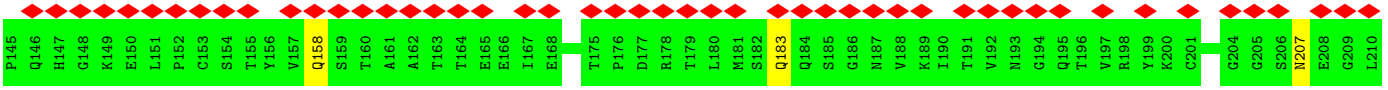


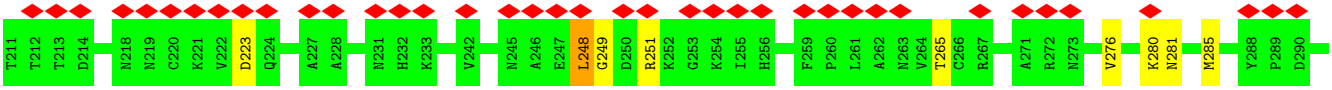


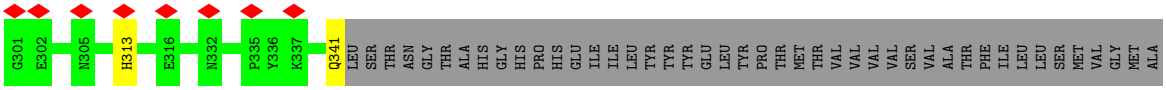
• Molecule 1: E1 envelope glycoprotein





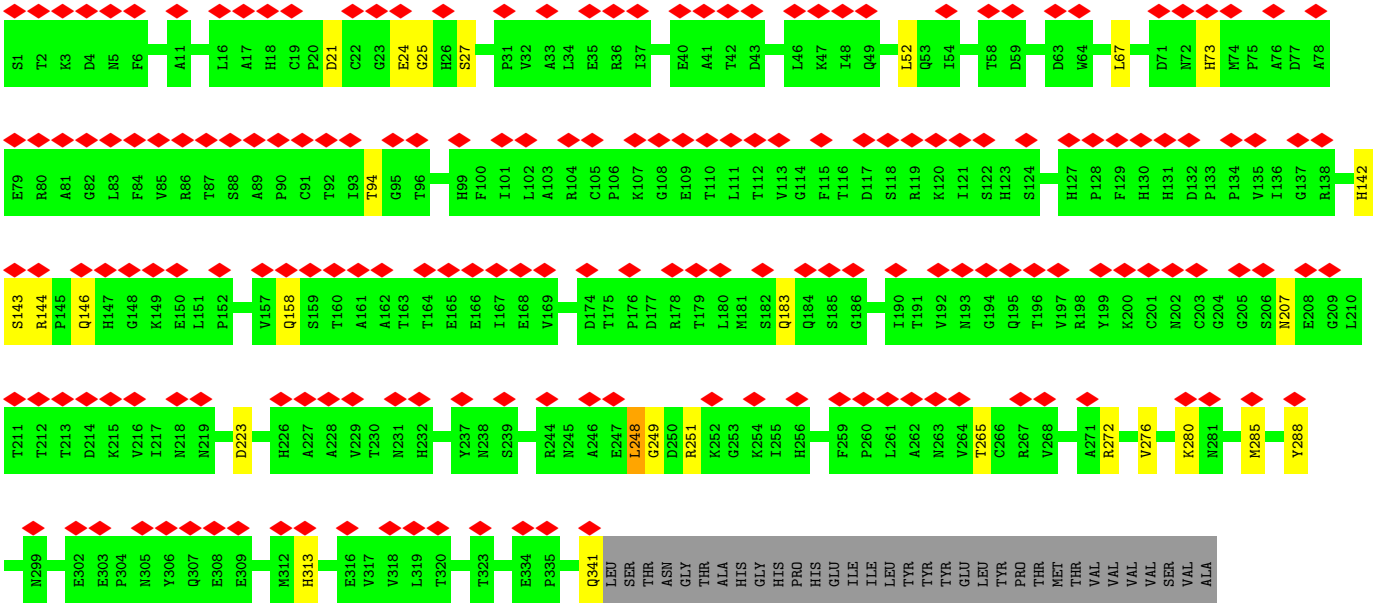






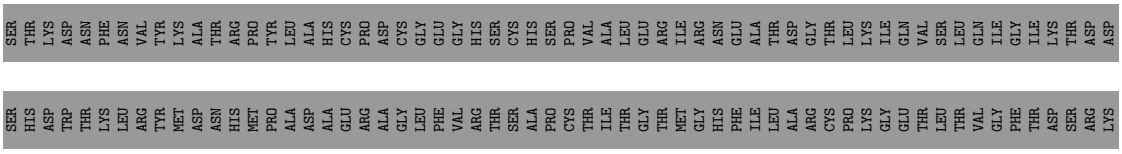
• Molecule 1: E1 envelope glycoprotein

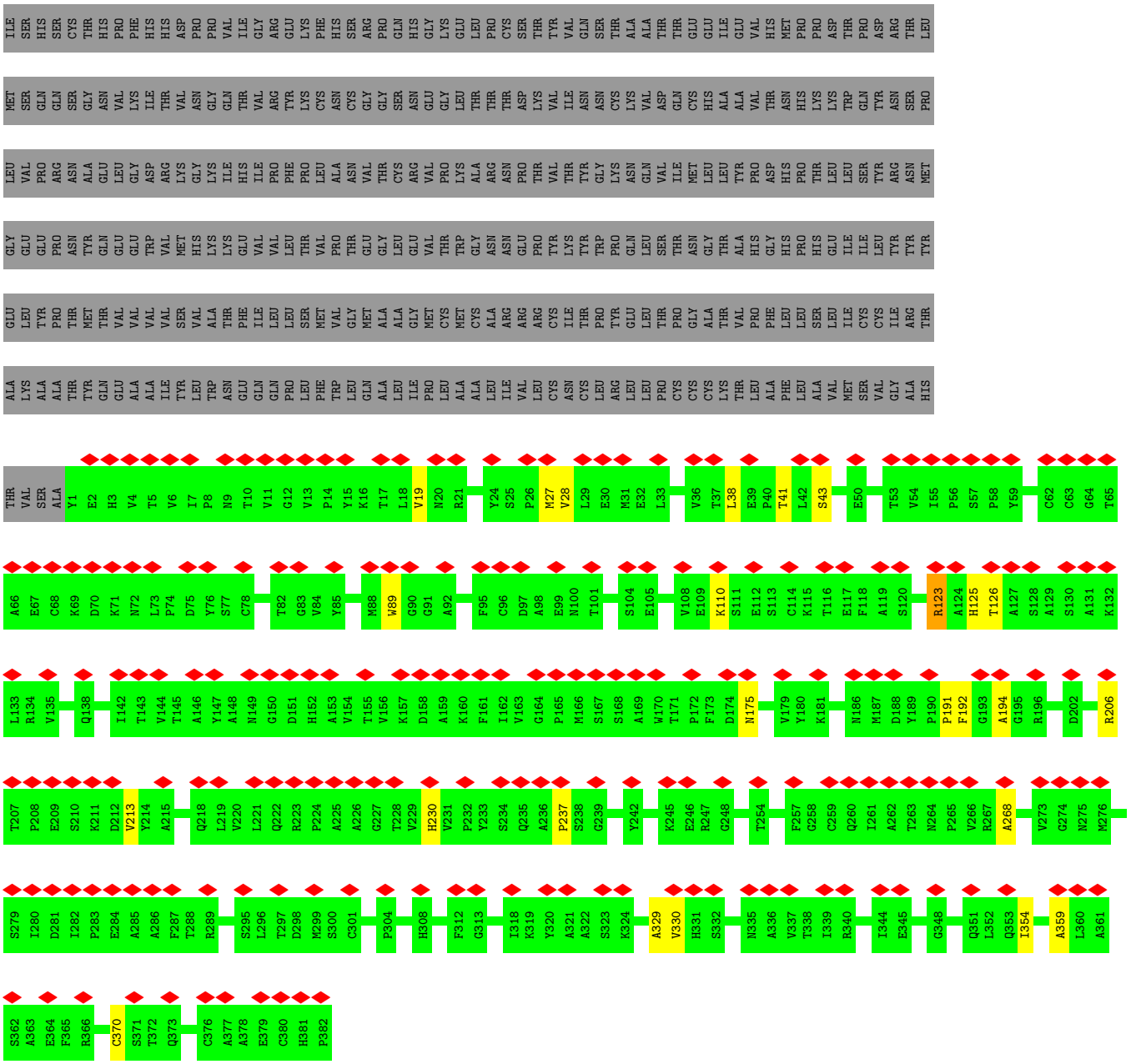
Chain B:



• Molecule 1: E1 envelope glycoprotein

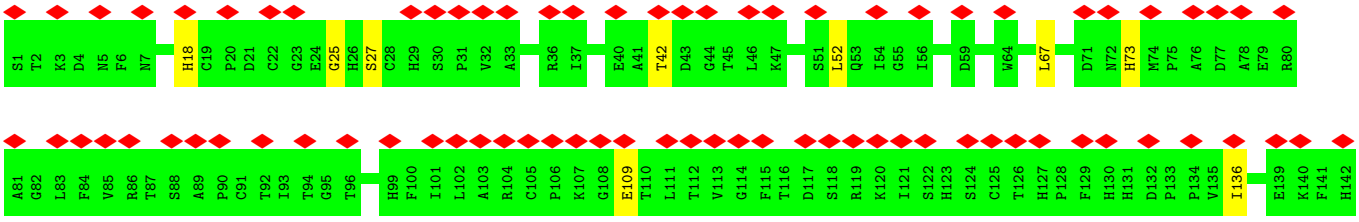
Chain N:

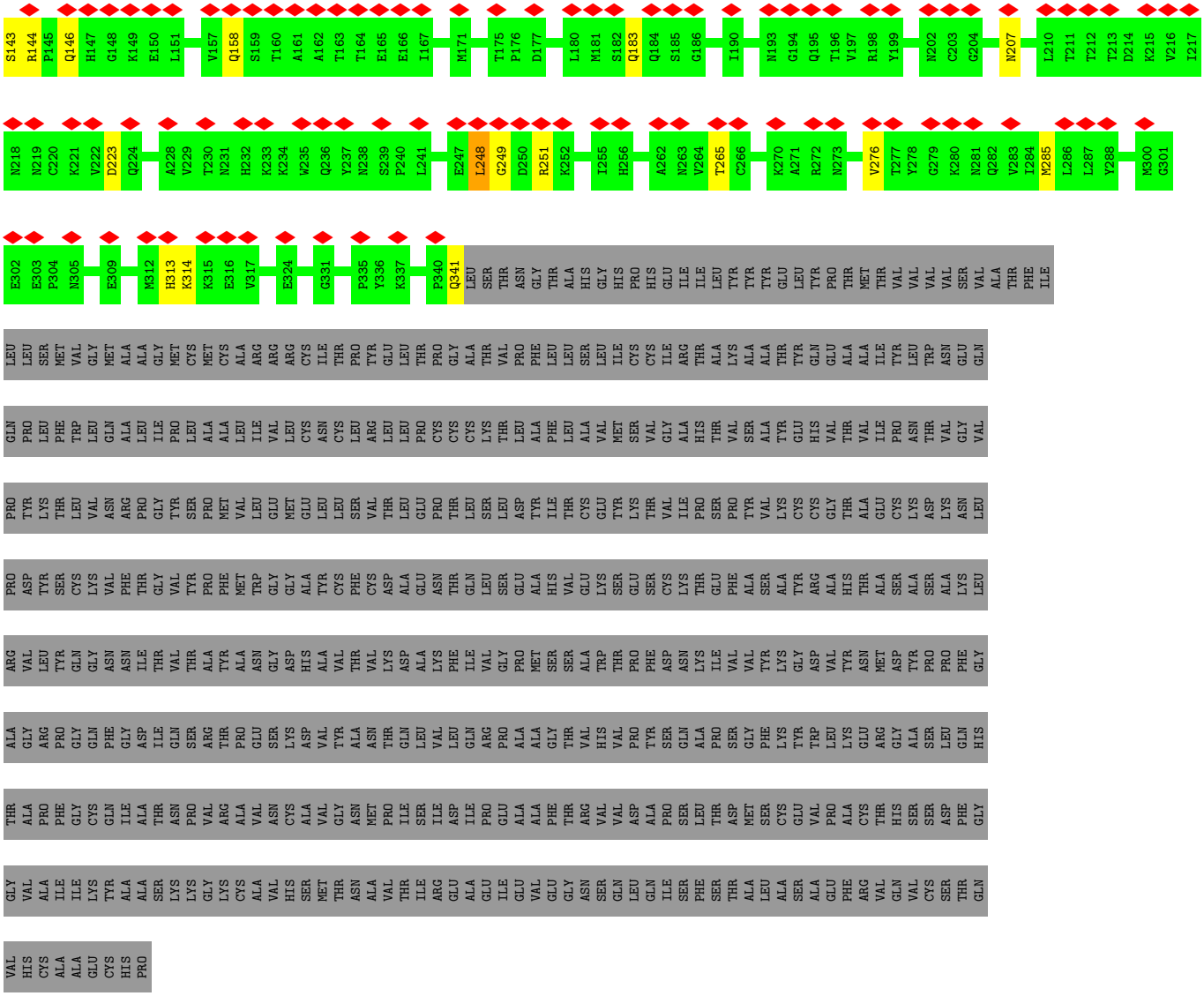




• Molecule 1: E1 envelope glycoprotein

Chain C:

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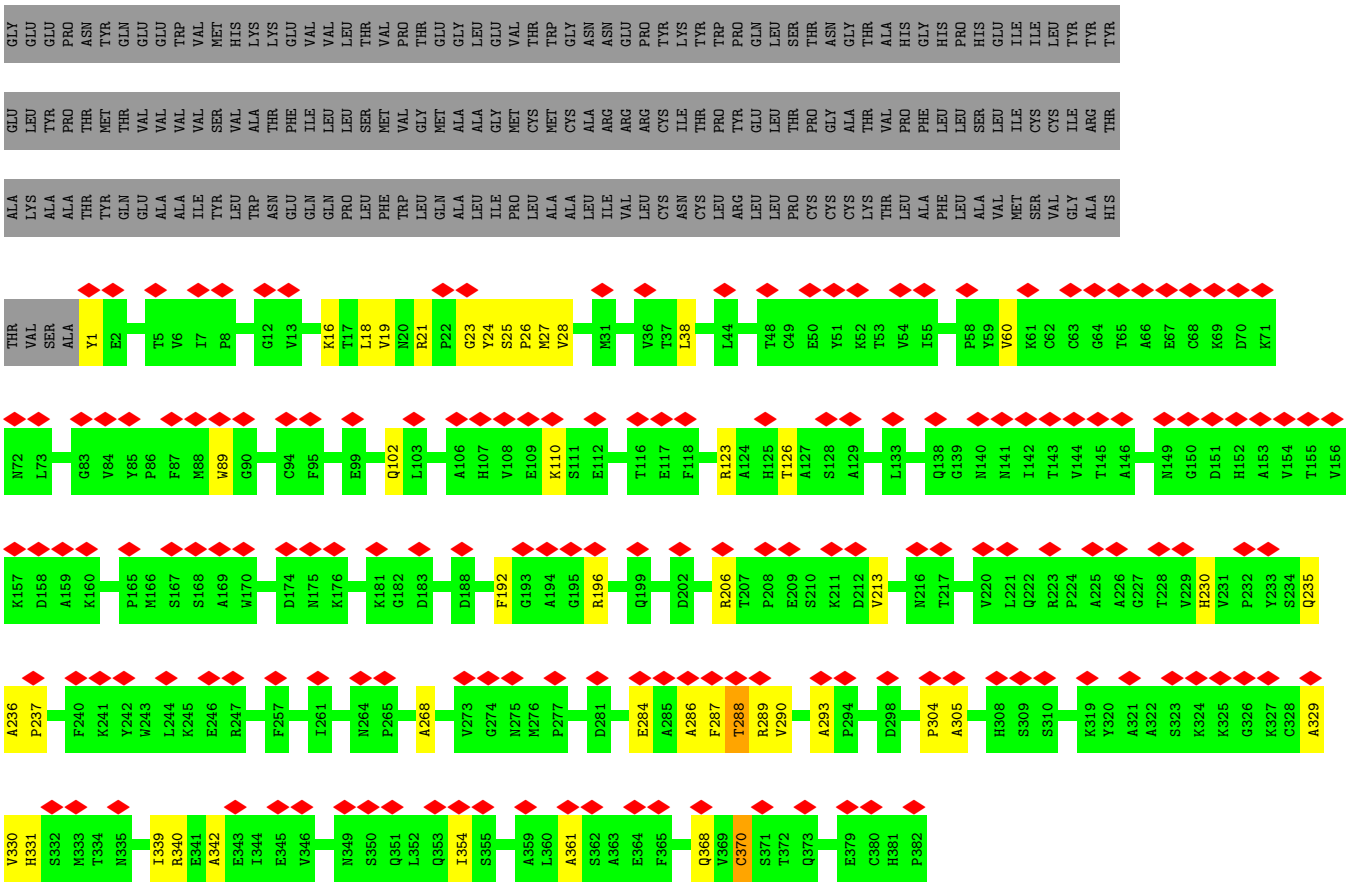
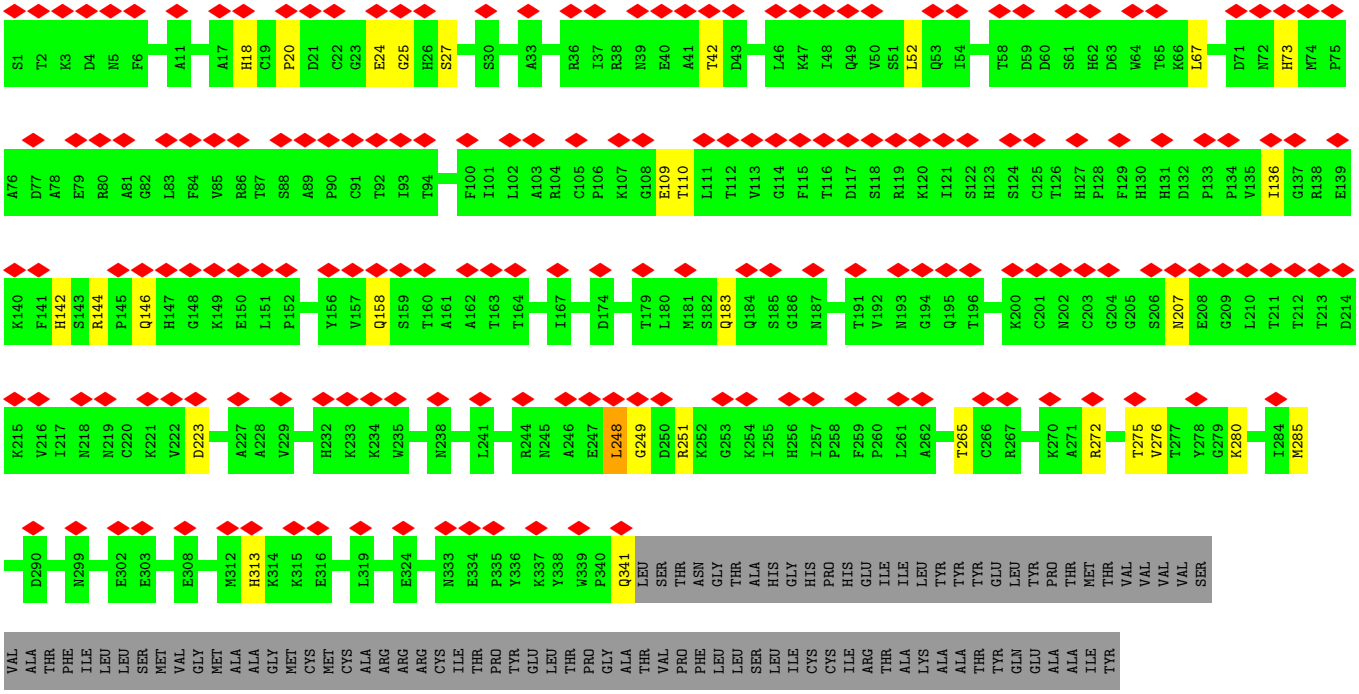
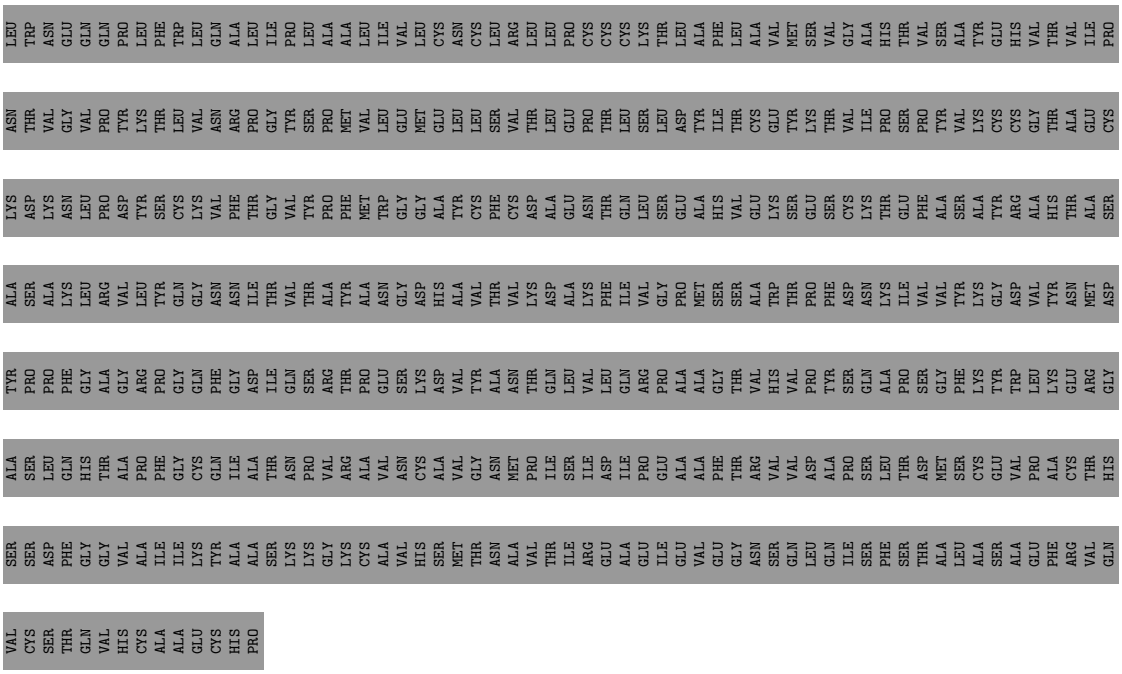
N218 N219 C220 K221 V222 D223 Q224 A228 V229 T230 N231 H232 K233 K234 W235 Q236 Y237 N238 S239 P240 L241 E247 L248 G249 D250 R251 K252 I255 H256 A262 N263 V264 T265 C266 K270 A271 R272 N273 V276 T277 Y278 G279 K280 N281 Q282 V283 I284 N285 L286 L287 Y288 M300 G301
E302 E303 P304 N305 E309 M312 H313 K314 K315 E316 V317 E324 G331 P335 Y336 K337 P340 Q341 LEU SER THR ASN GLY THR ALA HIS GLY HIS PRO HIS GLU ILE ILE LEU TYR TYR TYR GLU LEU TYR PRO THR MET THR VAL VAL VAL SER VAL ALA THR PHE ILE
LEU LEU SER MET VAL GLY MET ALA ALA GLY MET CYS MET CYS ALA ARG ARG ARG CYS ILE THR PRO TYR GLU LEU THR PRO GLY ALA THR VAL PRO PHE LEU LEU SER LEU ILE CYS CYS ILE ARG THR ALA LYS ALA ALA THR TYR GLN GLU ALA ALA ILE TYR LEU TRP ASN GLU GLN
GLN PRO LEU PHE TRP LEU GLN ALA LEU ILE PRO LEU ALA ALA LEU ILE VAL LEU CYS ASN CYS LEU ARG LEU LEU PRO CYS CYS CYS LYS THR LEU ALA PHE LEU ALA VAL MET SER VAL GLY ALA HIS THR VAL SER ALA TYR GLU HIS VAL THR VAL ILE PRO ASN THR VAL GLY VAL
PRO TYR LYS THR LEU VAL ASN ARG PRO GLY TYR SER PRO MET VAL LEU GLU MET GLU LEU LEU SER VAL THR LEU GLU PRO THR LEU SER LEU ASP TYR ILE THR CYS GLU TYR LYS THR VAL ILE PRO SER PRO TYR VAL LYS CYS CYS GLY THR ALA GLU CYS LYS ASP LYS ASN LEU
PRO ASP TYR SER CYS LYS VAL PHE THR GLY VAL TYR PRO PHE MET TRP GLY GLY ALA TYR CYS PHE CYS ASP ALA GLU ASN GLU LEU SER GLU SER ALA TRP THR PRO PHE ASP ASN LYS ILE VAL GLY PRO MET SER



• Molecule 1: E1 envelope glycoprotein

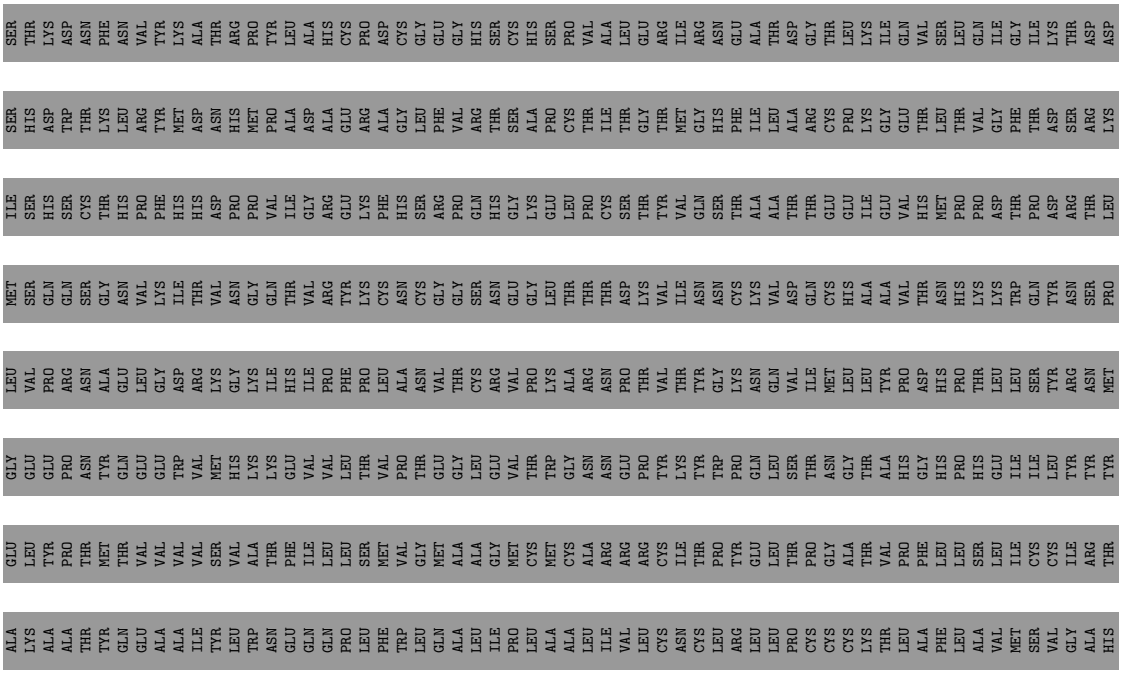
Chain D:

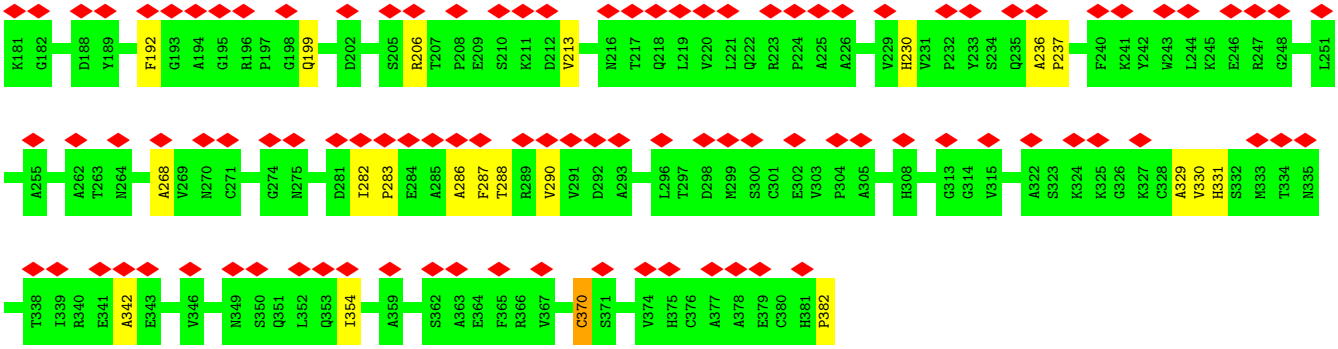




• Molecule 1: E1 envelope glycoprotein

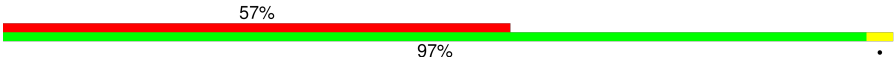
Chain P:

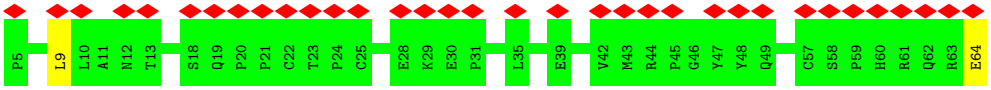




• Molecule 2: E3 envelope glycoprotein

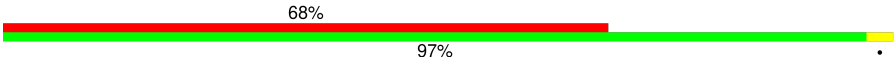
Chain U:

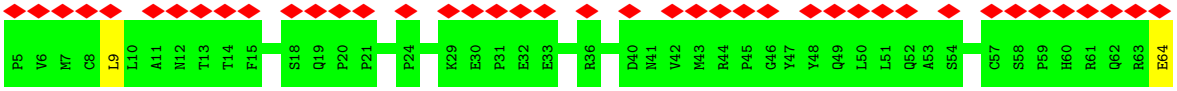




• Molecule 2: E3 envelope glycoprotein

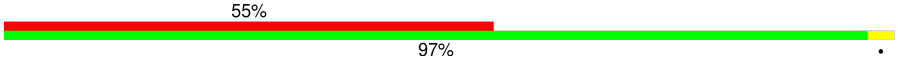
Chain V:

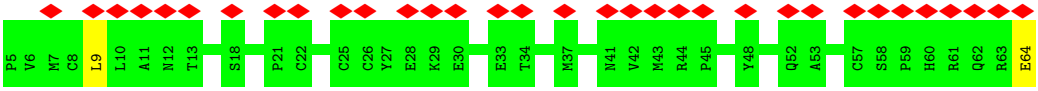




• Molecule 2: E3 envelope glycoprotein

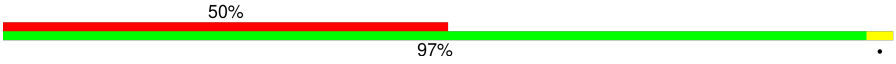
Chain W:

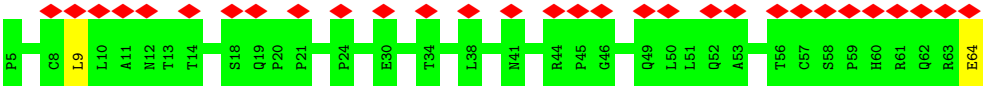




• Molecule 2: E3 envelope glycoprotein

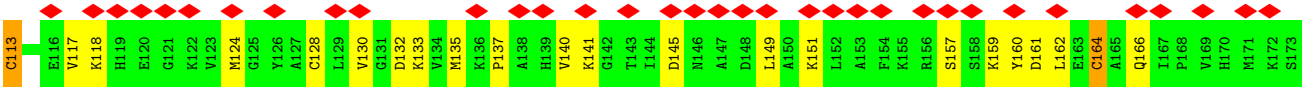
Chain X:

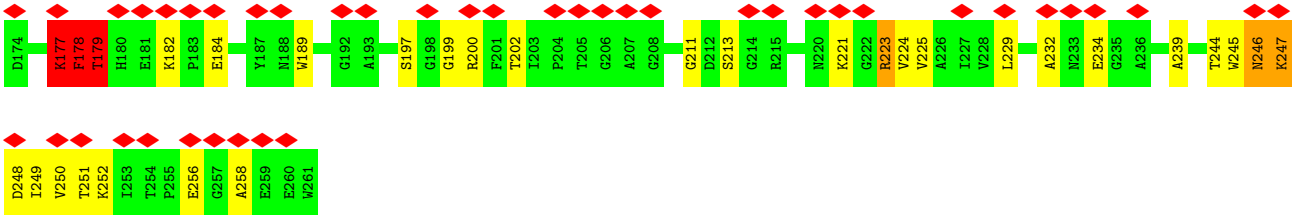




• Molecule 3: capsid protein

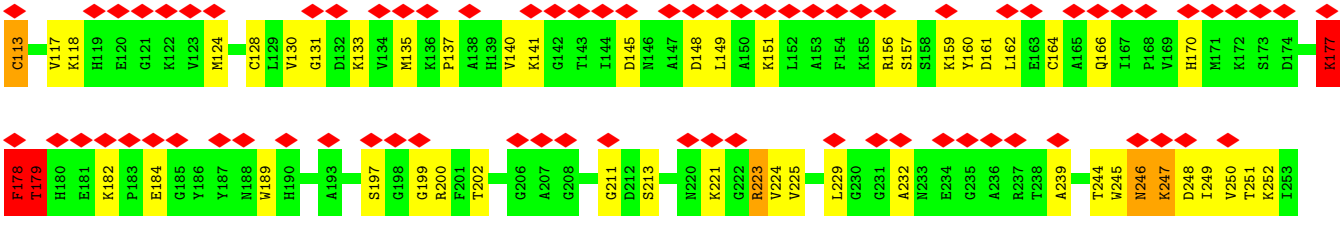
Chain I:





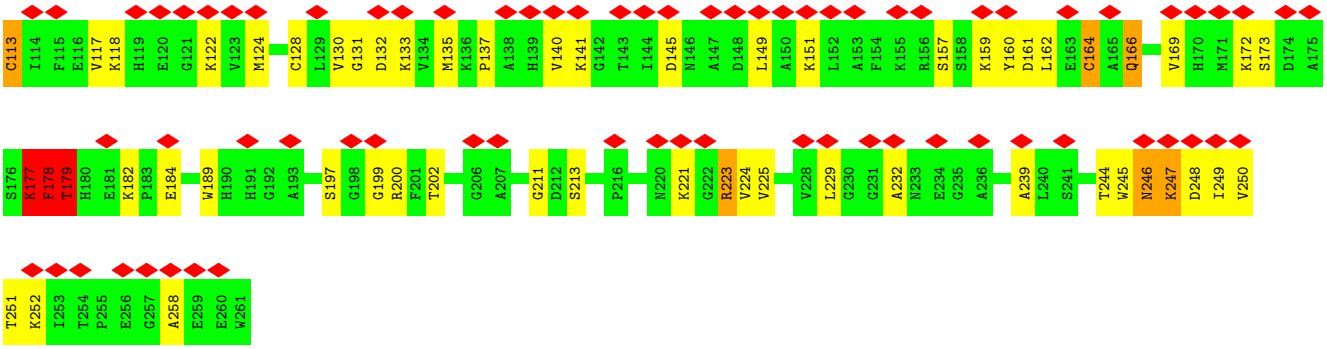
- Molecule 3: capsid protein

Chain J:



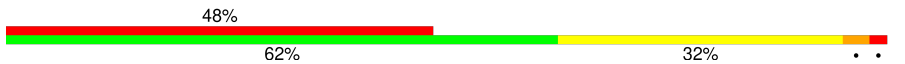
- Molecule 3: capsid protein

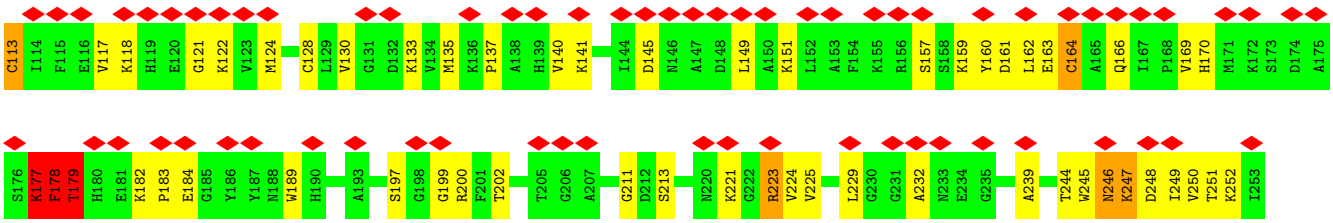
Chain K:

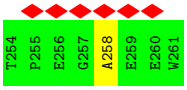


- Molecule 3: capsid protein

Chain L:

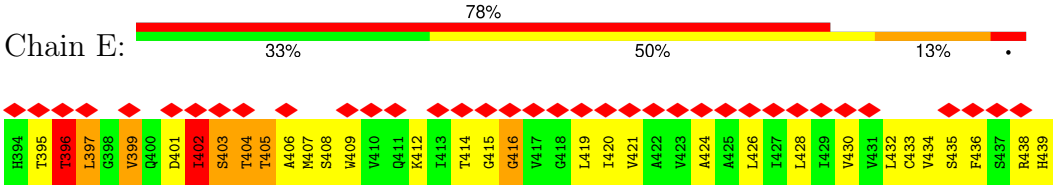






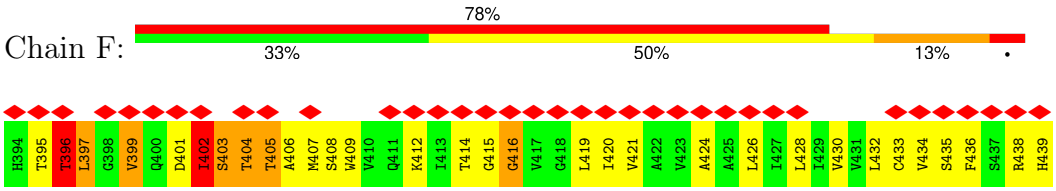
• Molecule 4: E1 envelope glycoprotein

Chain E:



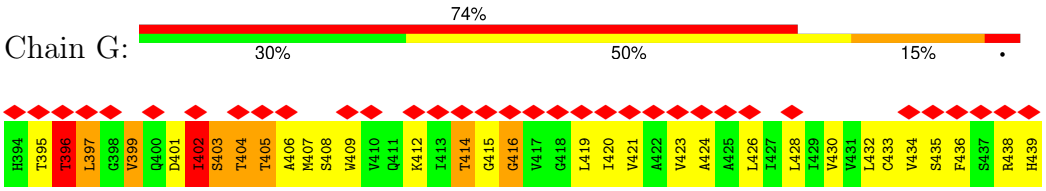
• Molecule 4: E1 envelope glycoprotein

Chain F:



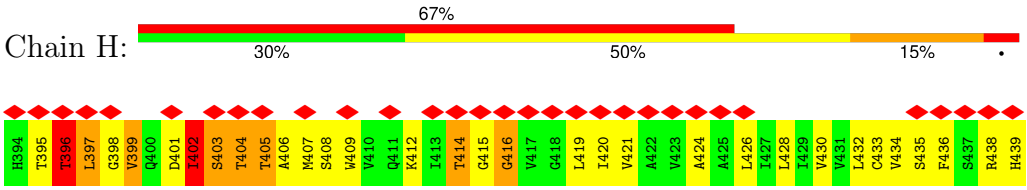
• Molecule 4: E1 envelope glycoprotein

Chain G:



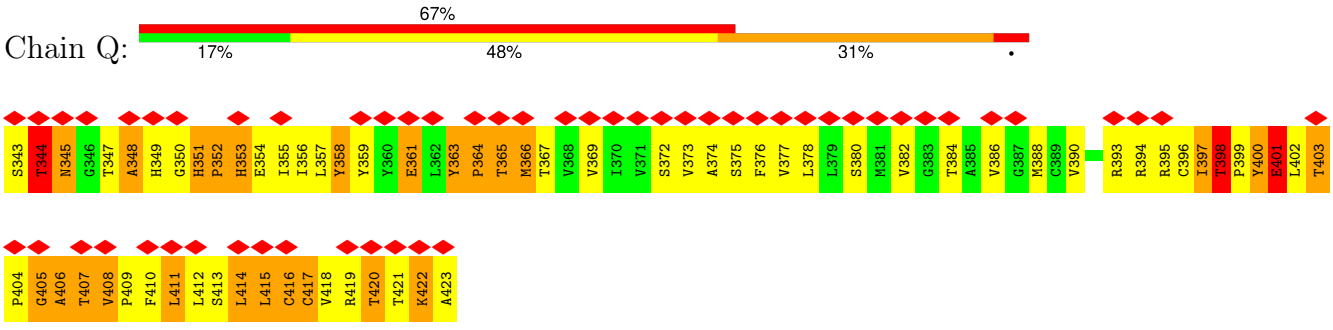
• Molecule 4: E1 envelope glycoprotein

Chain H:



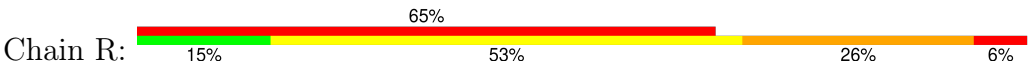
• Molecule 5: E2 envelope glycoprotein

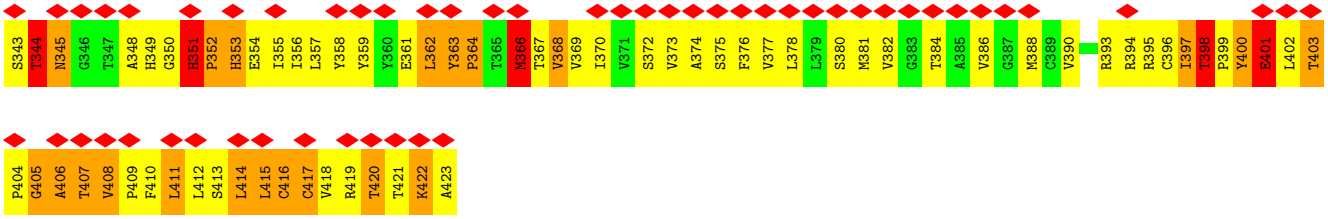
Chain Q:



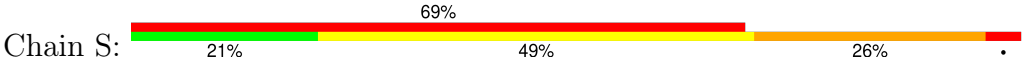
• Molecule 5: E2 envelope glycoprotein

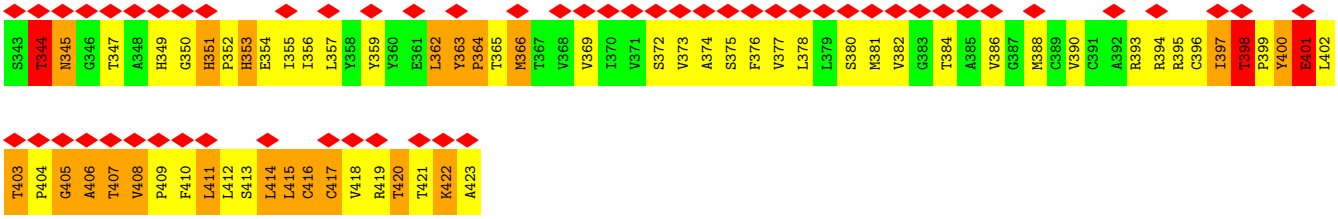
Chain R:



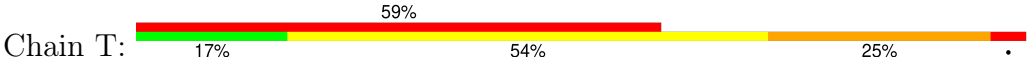


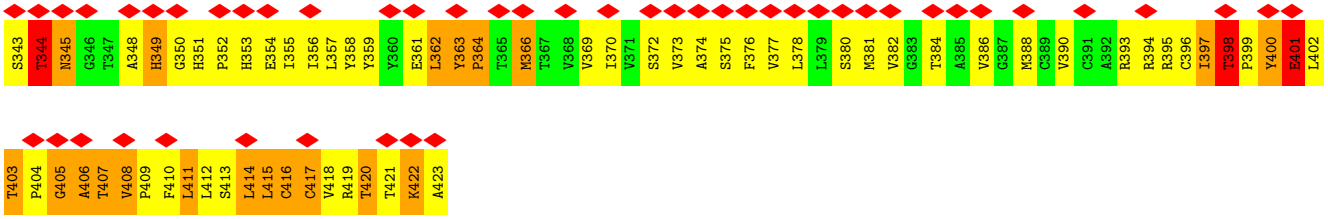
• Molecule 5: E2 envelope glycoprotein





• Molecule 5: E2 envelope glycoprotein





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72944	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 ($e^-/Å^2$)	36	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	5.000	Depositor
Minimum map value	-5.000	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.438	Depositor
Recommended contour level	1	Depositor
Map size (Å)	998.39996, 998.39996, 998.39996	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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	0.35	0/2763	0.58	0/3760
1	B	0.35	0/2763	0.58	0/3760
1	C	0.35	0/2763	0.58	0/3760
1	D	0.35	0/2763	0.59	0/3760
1	M	0.33	0/2984	0.57	0/4069
1	N	0.33	0/2984	0.57	0/4069
1	O	0.33	0/2984	0.57	0/4069
1	P	0.33	0/2984	0.57	0/4069
2	U	0.38	0/489	0.59	0/665
2	V	0.38	0/489	0.59	0/665
2	W	0.38	0/489	0.59	0/665
2	X	0.38	0/489	0.60	0/665
3	I	0.81	3/1169 (0.3%)	1.75	8/1577 (0.5%)
3	J	0.81	3/1169 (0.3%)	1.74	8/1577 (0.5%)
3	K	0.81	3/1169 (0.3%)	1.75	8/1577 (0.5%)
3	L	0.81	3/1169 (0.3%)	1.74	8/1577 (0.5%)
4	E	0.76	0/340	1.10	5/464 (1.1%)
4	F	0.76	0/340	1.10	5/464 (1.1%)
4	G	0.76	0/340	1.10	5/464 (1.1%)
4	H	0.76	0/340	1.10	5/464 (1.1%)
5	Q	0.34	0/627	0.49	0/858
5	R	0.33	0/627	0.48	0/858
5	S	0.33	0/627	0.48	0/858
5	T	0.32	0/627	0.46	0/858
All	All	0.46	12/33488 (0.0%)	0.86	52/45572 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	2
3	K	0	2
3	L	0	2
4	E	0	1
4	F	0	1
4	G	0	1
4	H	0	1
All	All	0	12

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	113	CYS	CB-SG	-14.10	1.58	1.82
3	K	113	CYS	CB-SG	-14.09	1.58	1.82
3	L	113	CYS	CB-SG	-14.03	1.58	1.82
3	I	113	CYS	CB-SG	-13.99	1.58	1.82
3	J	128	CYS	CB-SG	-12.10	1.61	1.82

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	177	LYS	O-C-N	-38.39	61.27	122.70
3	K	177	LYS	O-C-N	-38.37	61.31	122.70
3	L	177	LYS	O-C-N	-38.34	61.35	122.70
3	J	177	LYS	O-C-N	-38.34	61.35	122.70
3	J	178	PHE	O-C-N	-26.35	80.54	122.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	177	LYS	Mainchain
3	I	178	PHE	Mainchain
3	J	177	LYS	Mainchain
3	J	178	PHE	Mainchain
3	K	177	LYS	Mainchain

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	2691	0	2608	17	0
1	B	2691	0	2603	59	0
1	C	2691	0	2605	49	0
1	D	2691	0	2603	86	0
1	M	2911	0	2819	105	0
1	N	2911	0	2819	70	0
1	O	2911	0	2819	138	0
1	P	2911	0	2819	71	0
2	U	477	0	457	0	0
2	V	477	0	457	0	0
2	W	477	0	457	0	0
2	X	477	0	457	0	0
3	I	1141	0	1125	173	0
3	J	1141	0	1119	147	0
3	K	1141	0	1124	225	0
3	L	1141	0	1123	173	0
4	E	336	0	361	106	0
4	F	336	0	361	121	0
4	G	336	0	361	137	0
4	H	336	0	361	109	0
5	Q	613	0	630	348	0
5	R	613	0	631	368	0
5	S	613	0	629	404	0
5	T	613	0	631	357	0
All	All	32676	0	31979	2466	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 38.

The worst 5 of 2466 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)
3:J:160:TYR:CE2	5:R:398:THR:HG23	1.18	1.67
3:K:160:TYR:CZ	5:S:398:THR:HG23	1.24	1.65
3:I:160:TYR:CZ	5:Q:398:THR:HG23	1.27	1.64
4:H:402:ILE:HB	4:H:407:MET:SD	1.34	1.64
3:K:132:ASP:H	5:S:402:LEU:CD1	1.12	1.63

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	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	37	73
1	B	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	37	73
1	C	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	37	73
1	D	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	37	73
1	M	381/866 (44%)	370 (97%)	8 (2%)	3 (1%)	16	55
1	N	381/866 (44%)	372 (98%)	8 (2%)	1 (0%)	37	73
1	O	381/866 (44%)	370 (97%)	10 (3%)	1 (0%)	37	73
1	P	381/866 (44%)	370 (97%)	10 (3%)	1 (0%)	37	73
2	U	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
2	V	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
2	W	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
2	X	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
3	I	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	32
3	J	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	32
3	K	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	32
3	L	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	32
4	E	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	4
4	F	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	4
4	G	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	4
4	H	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	4
5	Q	79/81 (98%)	40 (51%)	15 (19%)	24 (30%)	0	0
5	R	79/81 (98%)	40 (51%)	15 (19%)	24 (30%)	0	0
5	S	79/81 (98%)	41 (52%)	17 (22%)	21 (27%)	0	0
5	T	79/81 (98%)	41 (52%)	20 (25%)	18 (23%)	0	1
All	All	4192/8272 (51%)	3808 (91%)	251 (6%)	133 (3%)	5	21

5 of 133 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	126	THR
1	N	126	THR
1	O	126	THR
1	P	126	THR
3	I	177	LYS

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	303/741 (41%)	294 (97%)	9 (3%)	36	55
1	B	303/741 (41%)	294 (97%)	9 (3%)	36	55
1	C	303/741 (41%)	294 (97%)	9 (3%)	36	55
1	D	303/741 (41%)	294 (97%)	9 (3%)	36	55
1	M	320/741 (43%)	316 (99%)	4 (1%)	65	77
1	N	320/741 (43%)	316 (99%)	4 (1%)	65	77
1	O	320/741 (43%)	315 (98%)	5 (2%)	58	74
1	P	320/741 (43%)	316 (99%)	4 (1%)	65	77
2	U	57/57 (100%)	55 (96%)	2 (4%)	31	51
2	V	57/57 (100%)	55 (96%)	2 (4%)	31	51
2	W	57/57 (100%)	55 (96%)	2 (4%)	31	51
2	X	57/57 (100%)	55 (96%)	2 (4%)	31	51
3	I	118/118 (100%)	109 (92%)	9 (8%)	11	30
3	J	118/118 (100%)	109 (92%)	9 (8%)	11	30
3	K	118/118 (100%)	109 (92%)	9 (8%)	11	30
3	L	118/118 (100%)	109 (92%)	9 (8%)	11	30
4	E	38/38 (100%)	37 (97%)	1 (3%)	41	59
4	F	38/38 (100%)	37 (97%)	1 (3%)	41	59
4	G	38/38 (100%)	37 (97%)	1 (3%)	41	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	38/38 (100%)	37 (97%)	1 (3%)	41 59
5	Q	70/70 (100%)	63 (90%)	7 (10%)	6 20
5	R	70/70 (100%)	61 (87%)	9 (13%)	3 14
5	S	70/70 (100%)	63 (90%)	7 (10%)	6 20
5	T	70/70 (100%)	61 (87%)	9 (13%)	3 14
All	All	3624/7060 (51%)	3491 (96%)	133 (4%)	31 49

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	397	LEU
5	S	363	TYR
5	T	398	THR
1	D	73	HIS
2	X	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	246	ASN
3	L	233	ASN
3	L	246	ASN
3	K	246	ASN
1	O	138	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 oligosaccharides 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.

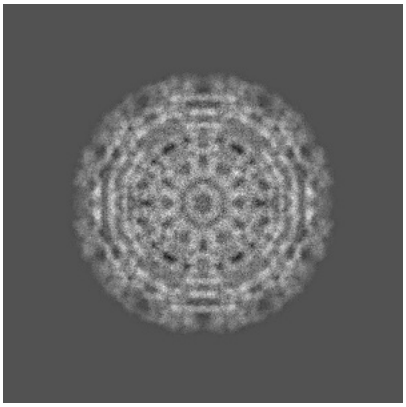
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8734. These allow visual inspection of the internal detail of the map and identification of artifacts.

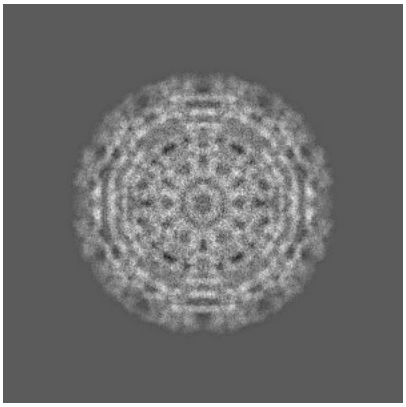
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

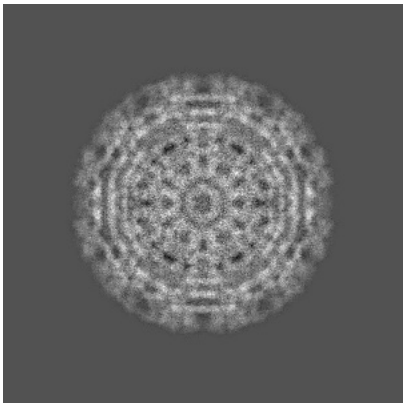
6.1.1 Primary map



X



Y

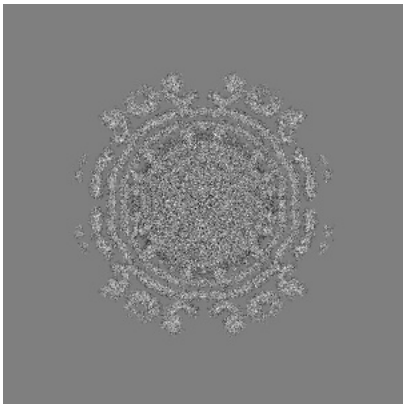


Z

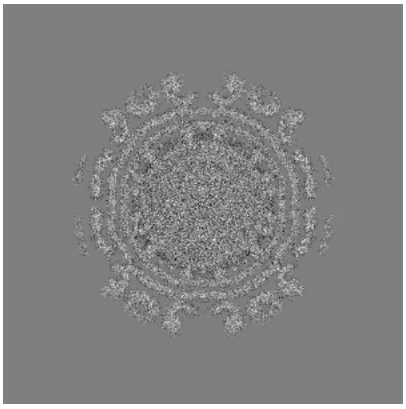
The images above show the map projected in three orthogonal directions.

6.2 Central slices

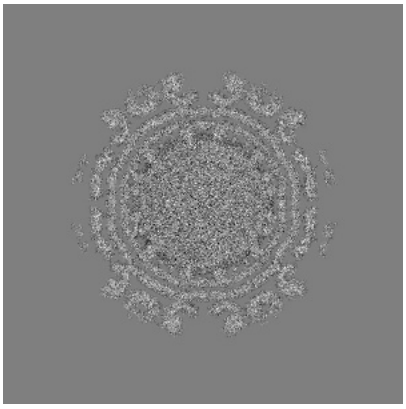
6.2.1 Primary map



X Index: 384



Y Index: 384

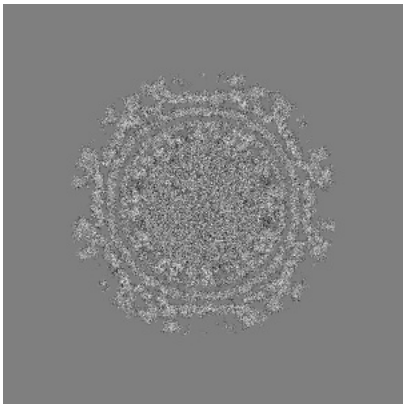


Z Index: 384

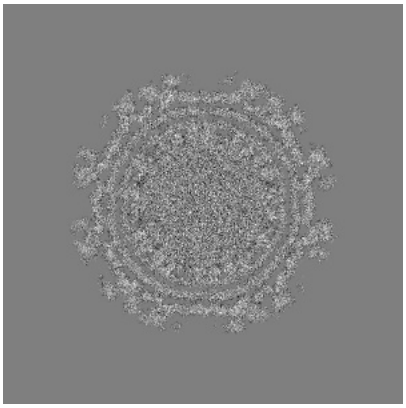
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

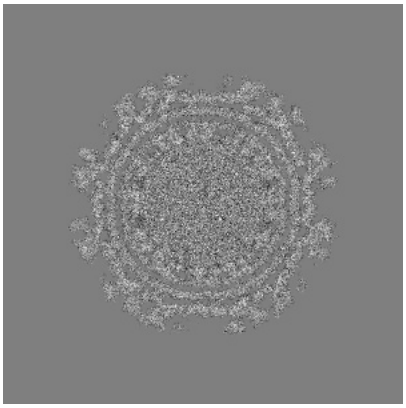
6.3.1 Primary map



X Index: 362



Y Index: 405

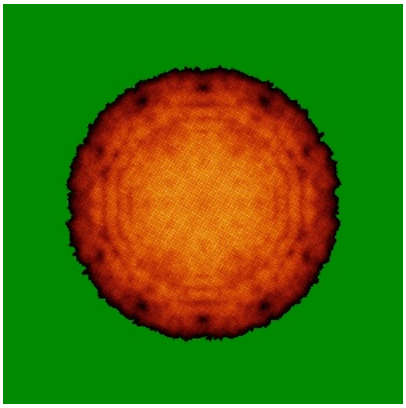


Z Index: 406

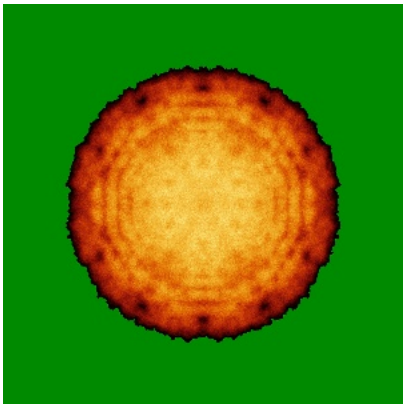
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

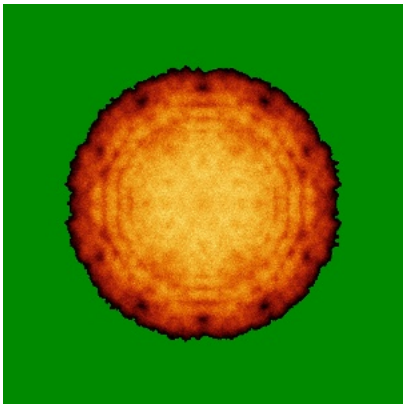
6.4.1 Primary map



X



Y

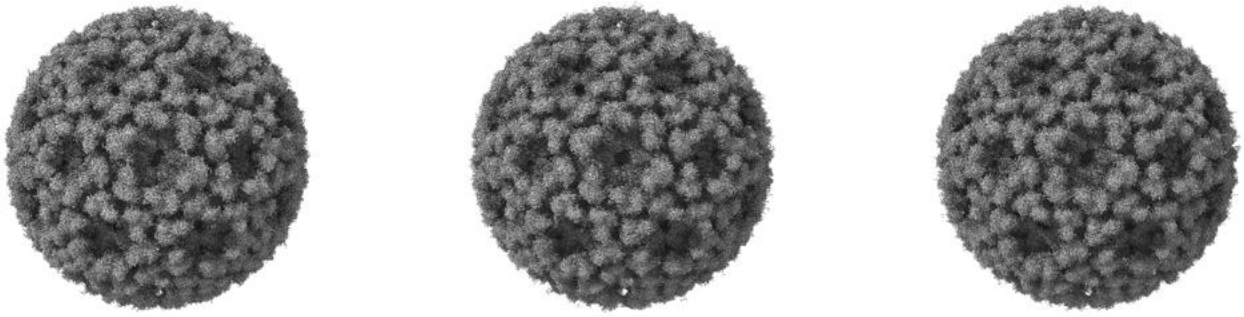


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

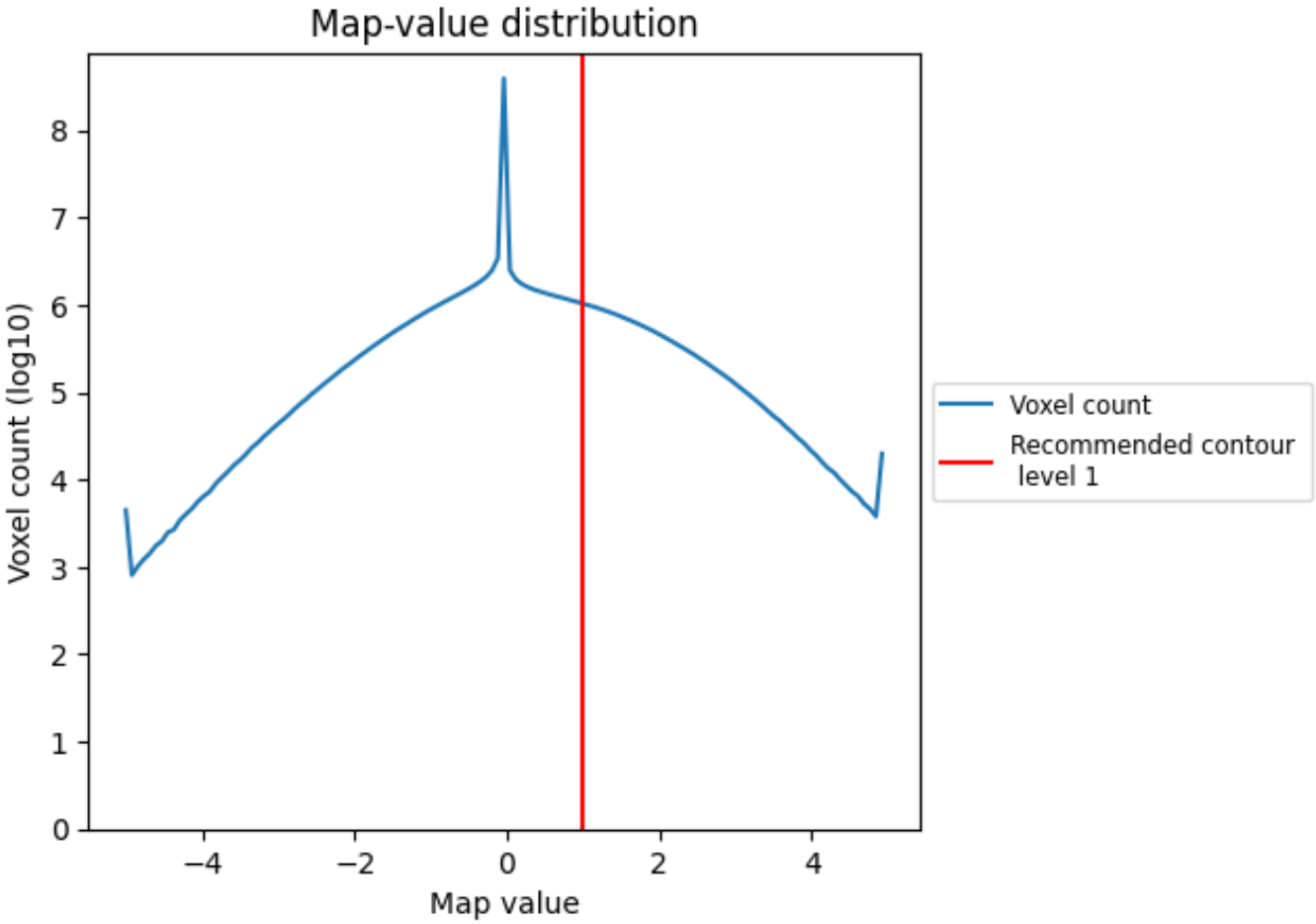
6.6 Mask visualisation (i)

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

7 Map analysis

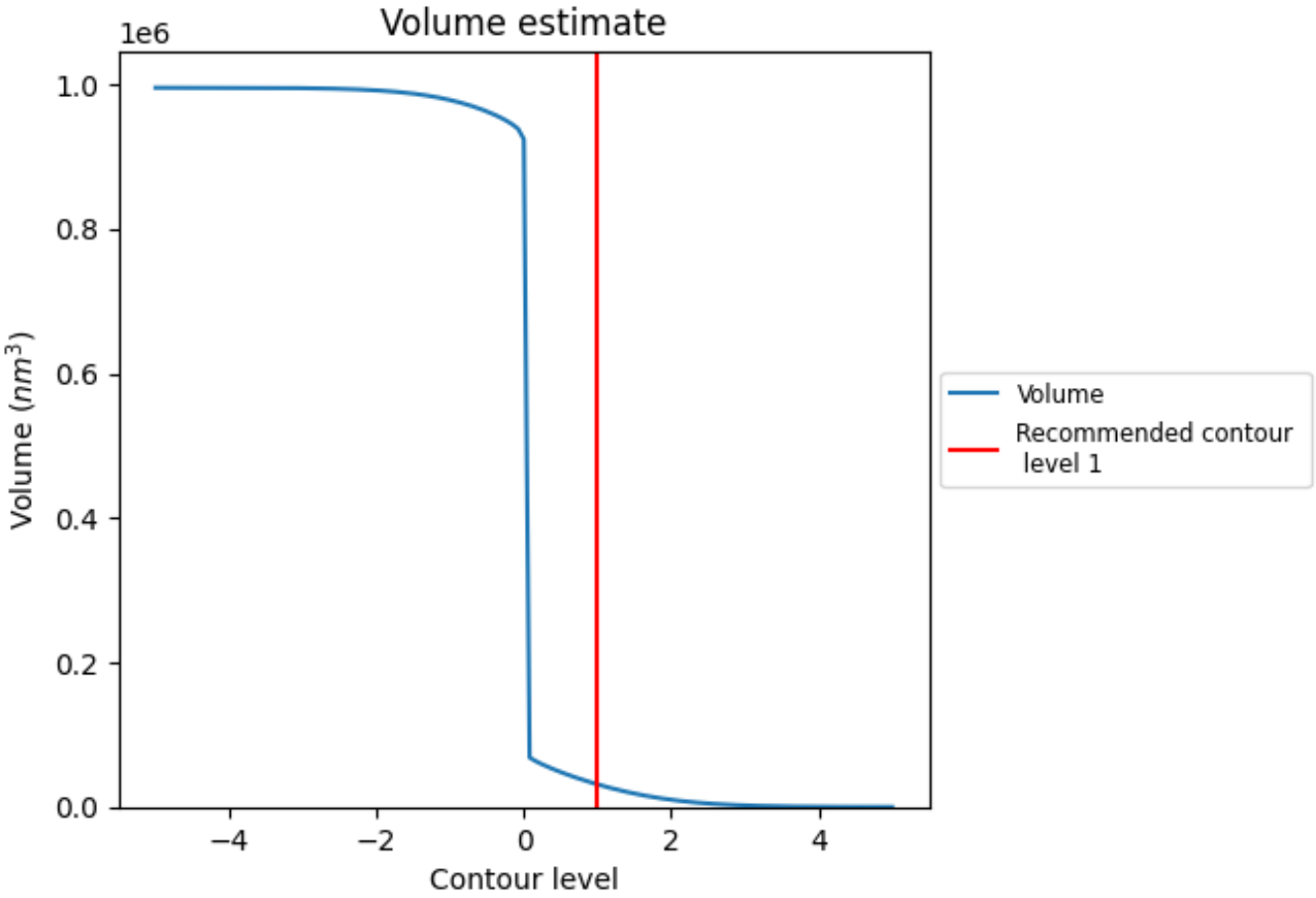
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

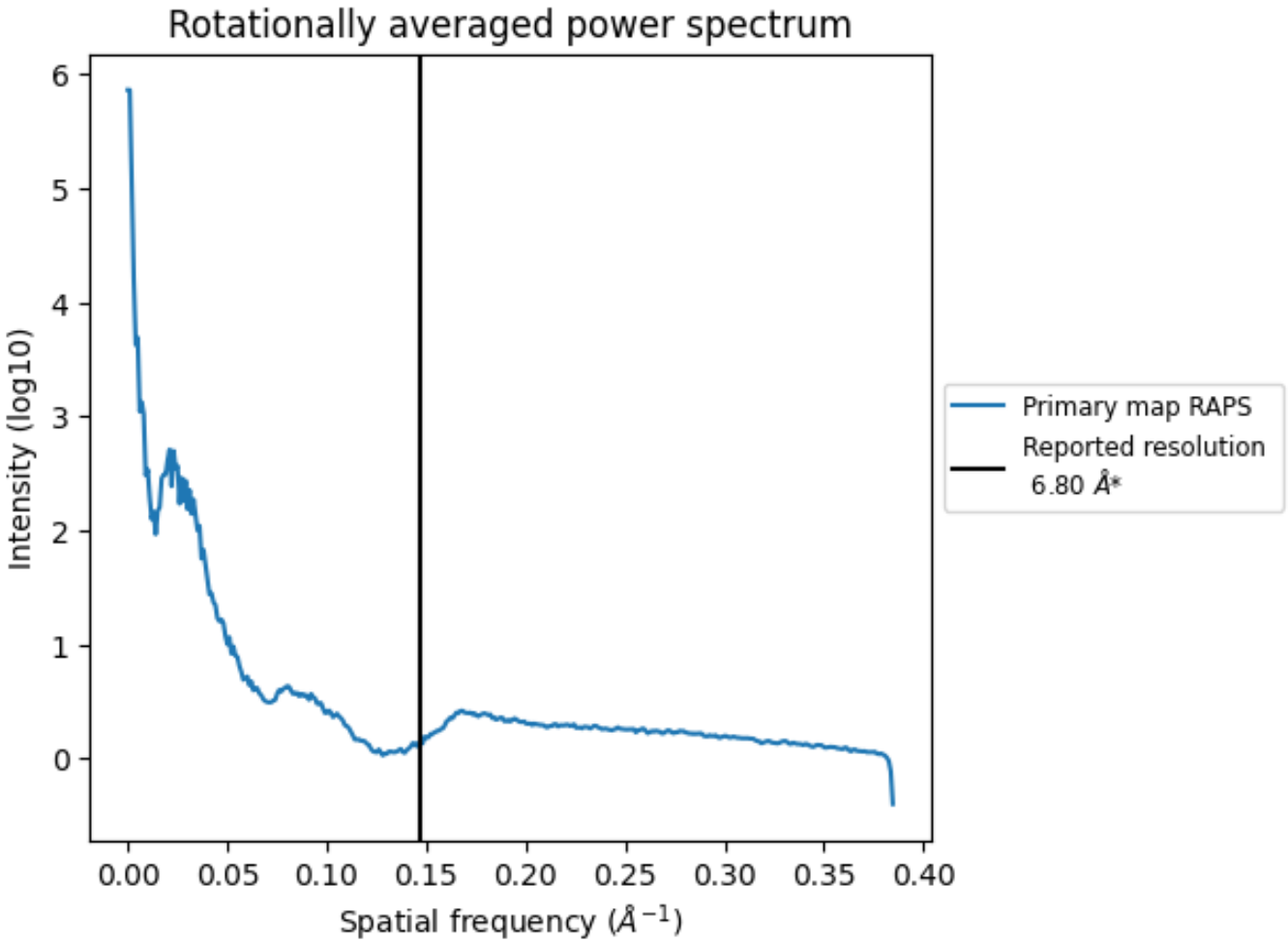
7.2 Volume estimate (i)



The volume at the recommended contour level is 31225 nm^3; this corresponds to an approximate mass of 28206 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)

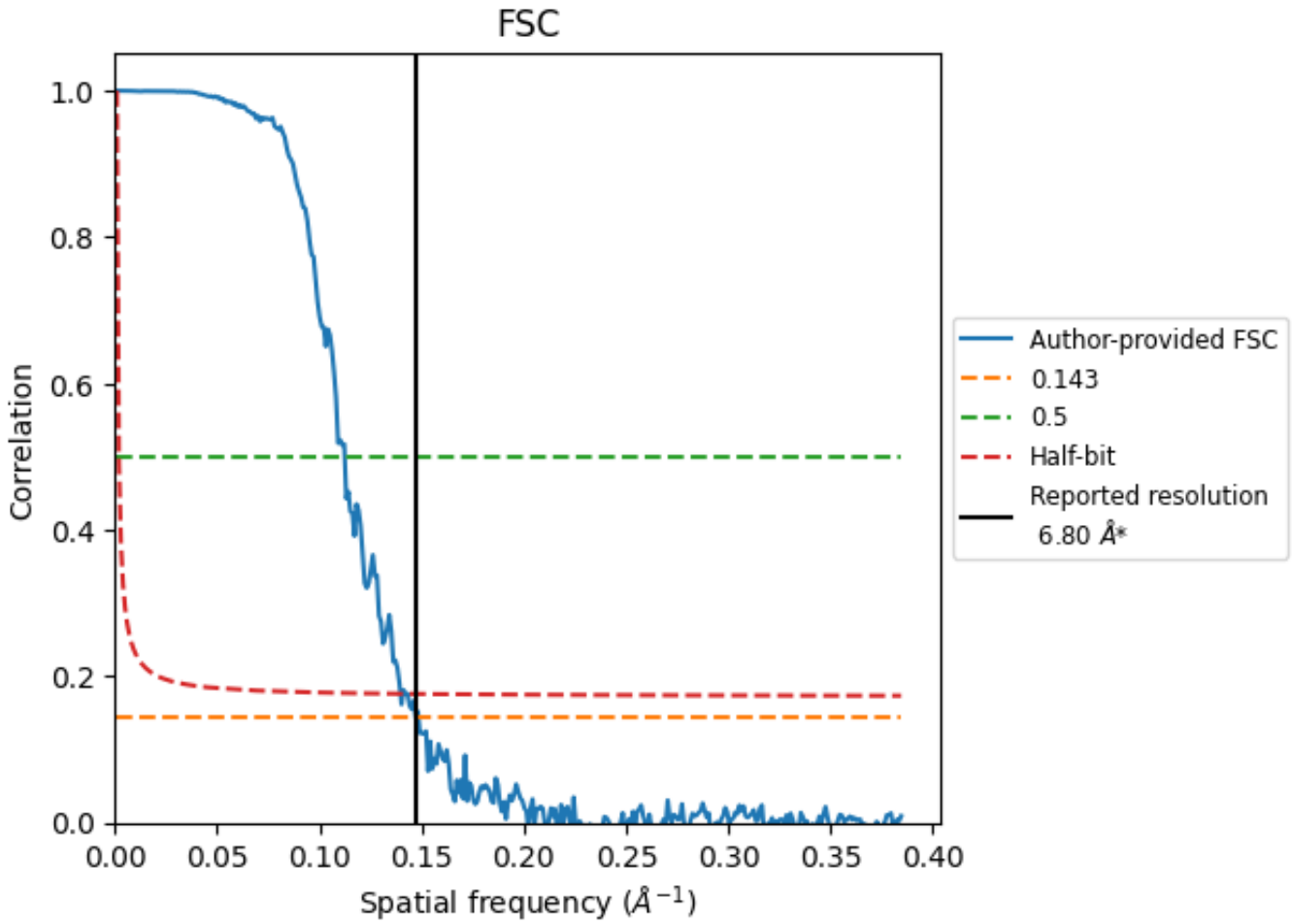


*Reported resolution corresponds to spatial frequency of 0.147 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.147 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.79	8.90	7.16
Unmasked-calculated*	-	-	-

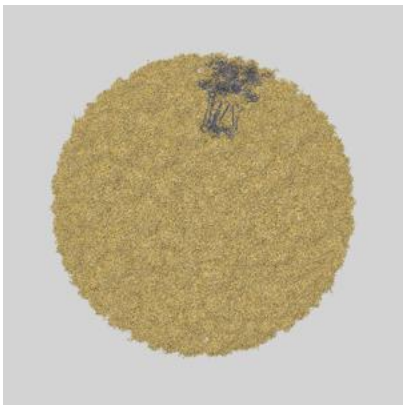
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

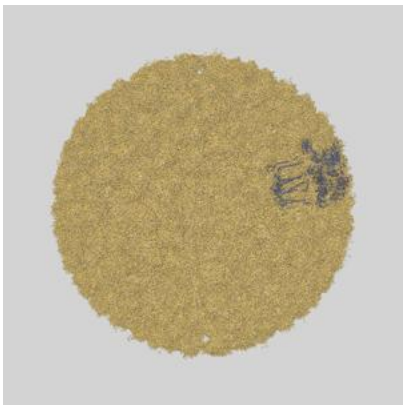
This section contains information regarding the fit between EMDB map EMD-8734 and PDB model 5VU2. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

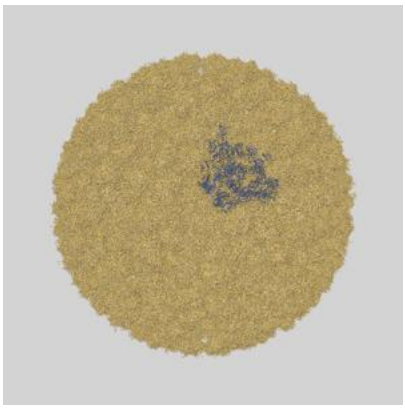
9.1.1 Map-model overlay



X

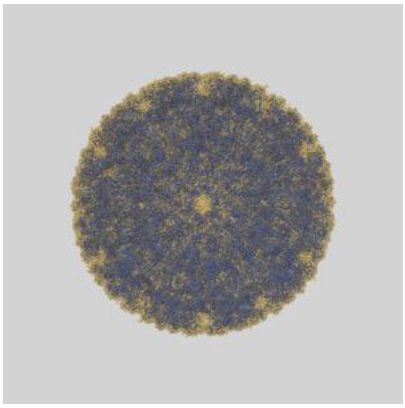


Y

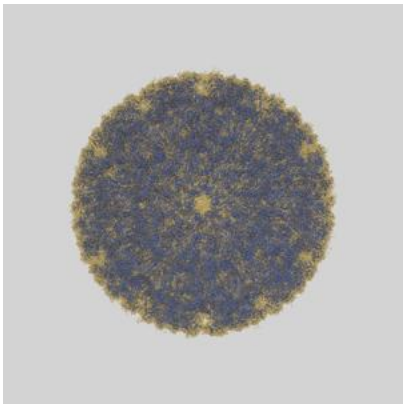


Z

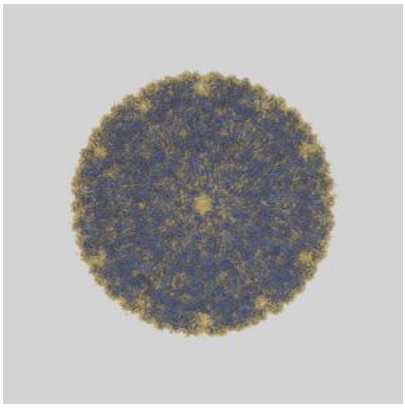
9.1.2 Map-model assembly overlay



X



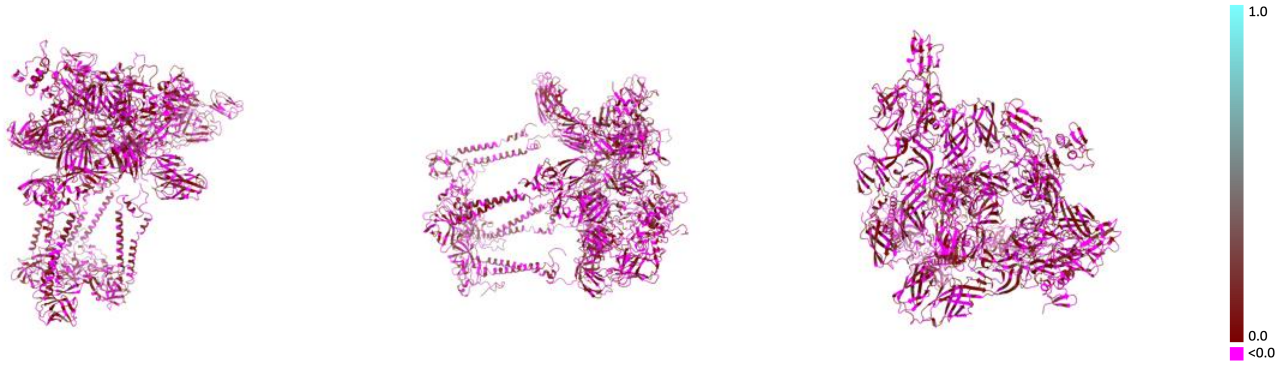
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

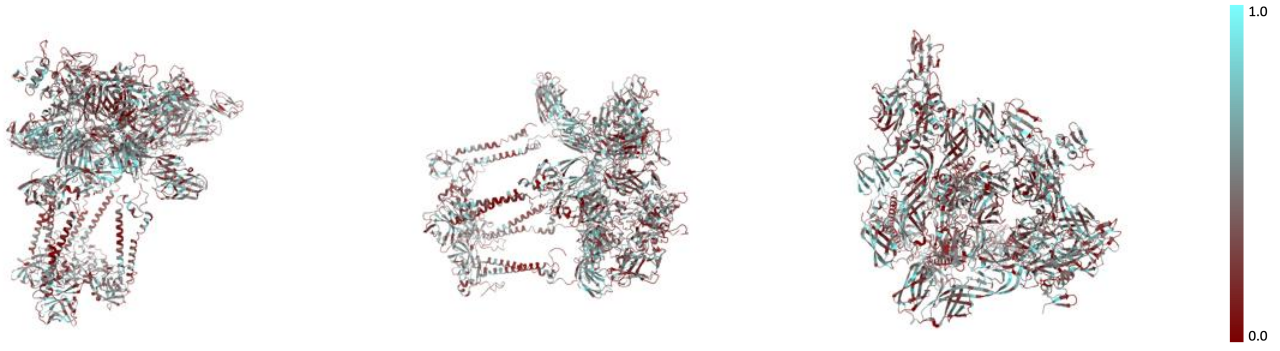
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

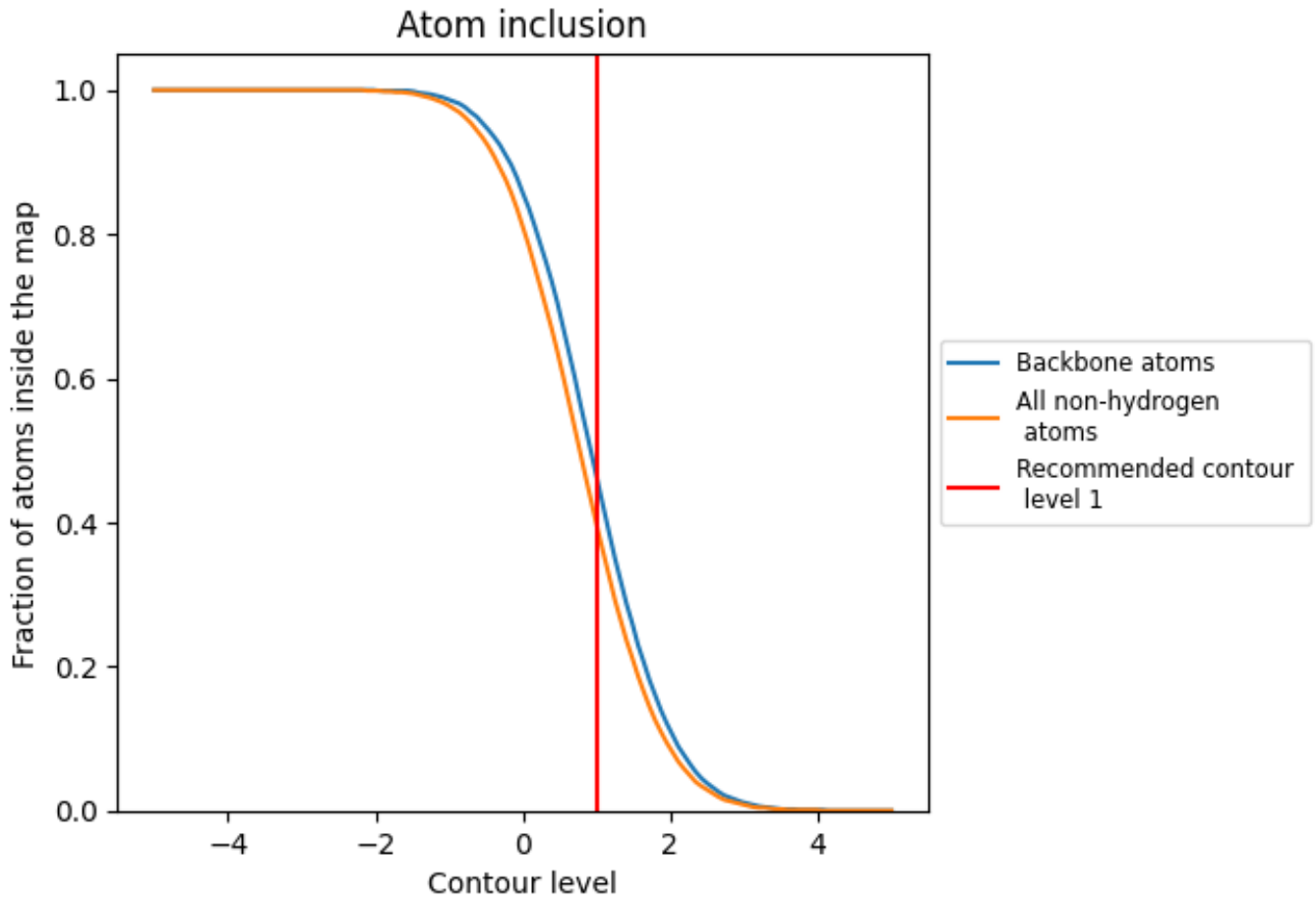
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 40% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3960	0.0260
A	0.4020	0.0200
B	0.3780	0.0280
C	0.3990	0.0320
D	0.3970	0.0170
E	0.2340	0.0110
F	0.2700	-0.0000
G	0.2550	0.0270
H	0.2670	0.0410
I	0.4030	0.0230
J	0.3990	0.0310
K	0.4060	0.0420
L	0.4090	0.0280
M	0.4430	0.0360
N	0.3780	0.0180
O	0.4520	0.0360
P	0.4680	0.0290
Q	0.3030	0.0130
R	0.3100	0.0250
S	0.2800	0.0230
T	0.3500	0.0540
U	0.3600	-0.0090
V	0.2730	-0.0140
W	0.3910	-0.0000
X	0.4210	0.0210