



wwPDB EM Validation Summary Report ⓘ

May 29, 2025 – 05:08 pm BST

PDB ID : 9H2H / pdb_00009h2h
EMDB ID : EMD-51803
Title : AcMNPV apical cap - composite map of the C2 plug
Authors : Effantin, G.; Kandiah, E.; Pelosse, M.
Deposited on : 2024-10-11
Resolution : 6.10 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

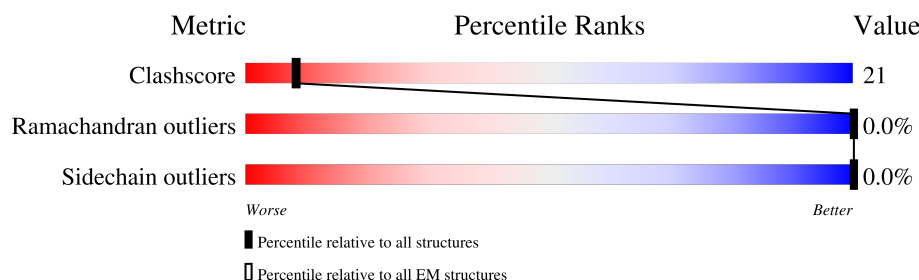
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.10 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 $\leq 5\%$. 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	365	<div> <div>6%</div> <div>56%</div> <div>35%</div> <div>9%</div> </div>
1	B	365	<div> <div>5%</div> <div>54%</div> <div>39%</div> <div>8%</div> </div>
1	C	365	<div> <div>52%</div> <div>37%</div> <div>11%</div> </div>
1	D	365	<div> <div>50%</div> <div>39%</div> <div>11%</div> </div>
2	E	58	<div> <div>9%</div> <div>91%</div> </div>
3	F	58	<div> <div>100%</div> </div>
4	G	290	<div> <div>14%</div> <div>49%</div> <div>34%</div> <div>17%</div> </div>
4	H	290	<div> <div>14%</div> <div>39%</div> <div>16%</div> <div>45%</div> </div>

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Mol	Chain	Length	Quality of chain
4	K	290	
4	L	290	
4	O	290	
4	P	290	
4	S	290	
4	T	290	
5	I	361	
5	J	361	
5	M	361	
5	N	361	
5	Q	361	
5	R	361	
5	U	361	
5	V	361	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39098 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 Protein AC54.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	332	Total	C	N	O	S	0	0
			2717	1723	479	497	18		
1	B	337	Total	C	N	O	S	0	0
			2757	1752	484	502	19		
1	C	324	Total	C	N	O	S	0	0
			2660	1691	468	483	18		
1	D	325	Total	C	N	O	S	0	0
			2666	1700	469	478	19		

- Molecule 2 is a DNA chain called DNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	58	Total	C	N	O	P	0	0
			1198	574	233	333	58		

- Molecule 3 is a DNA chain called DNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	58	Total	C	N	O	P	0	0
			1177	573	186	361	57		

- Molecule 4 is a protein called Occlusion-derived virus envelope protein E27.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	240	Total	C	N	O	S	0	0
			1941	1247	312	373	9		
4	H	160	Total	C	N	O	S	0	0
			1301	844	215	234	8		
4	K	228	Total	C	N	O	S	0	0
			1850	1191	296	354	9		
4	L	130	Total	C	N	O	S	0	0
			1061	692	172	190	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	238	Total	C	N	O	S	0	0
			1926	1238	309	370	9		
4	P	160	Total	C	N	O	S	0	0
			1302	847	212	235	8		
4	S	222	Total	C	N	O	S	0	0
			1805	1164	284	349	8		
4	T	178	Total	C	N	O	S	0	0
			1440	938	234	260	8		

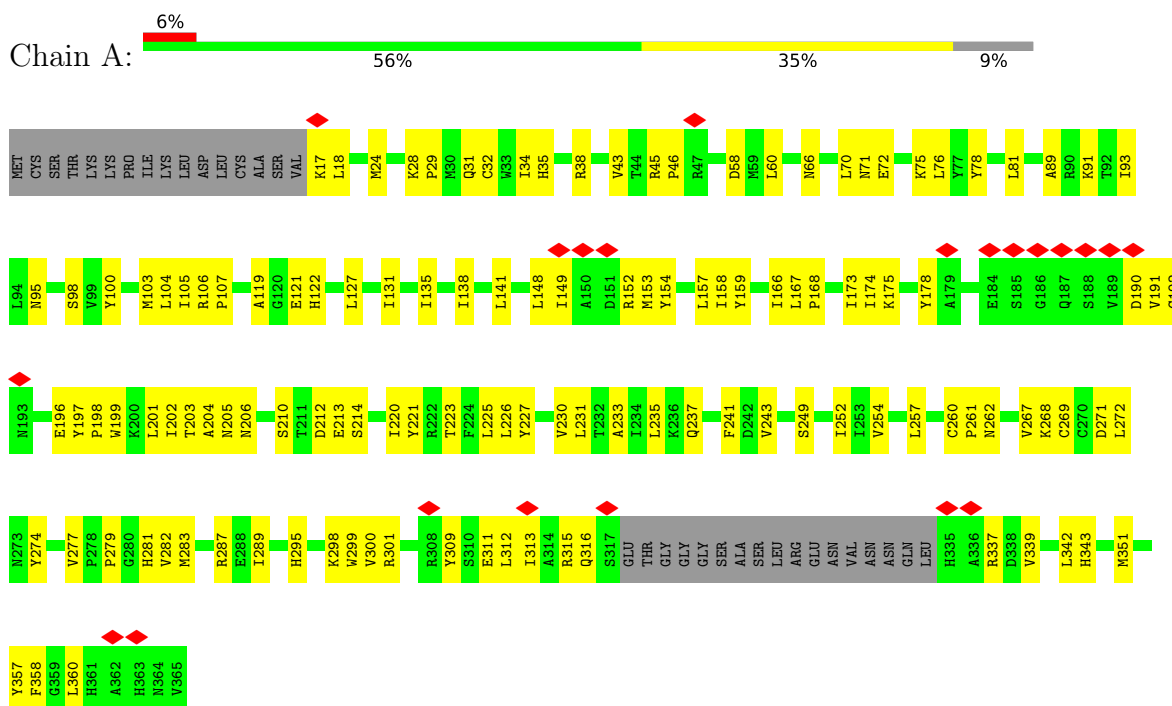
- Molecule 5 is a protein called Protein C42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	213	Total	C	N	O	S	0	0
			1760	1117	296	331	16		
5	J	194	Total	C	N	O	S	0	0
			1622	1033	275	301	13		
5	M	213	Total	C	N	O	S	0	0
			1760	1117	296	331	16		
5	N	181	Total	C	N	O	S	0	0
			1517	966	257	282	12		
5	Q	213	Total	C	N	O	S	0	0
			1760	1117	296	331	16		
5	R	178	Total	C	N	O	S	0	0
			1488	943	253	279	13		
5	U	213	Total	C	N	O	S	0	0
			1760	1117	296	331	16		
5	V	196	Total	C	N	O	S	0	0
			1630	1036	276	306	12		

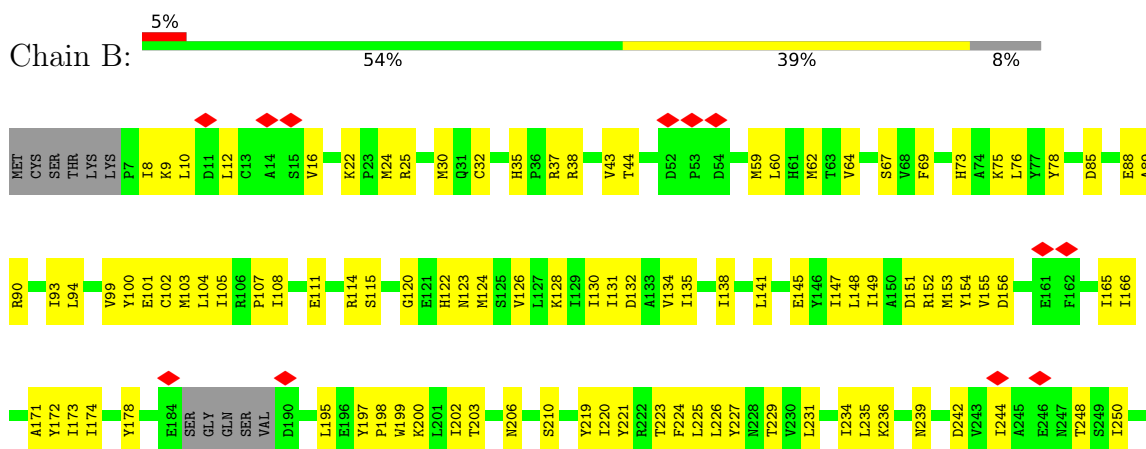
3 Residue-property plots

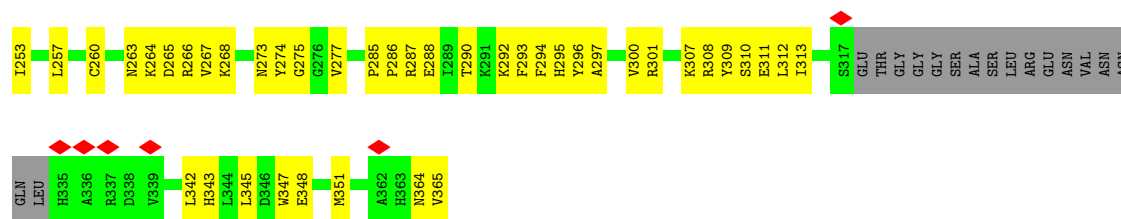
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Protein AC54



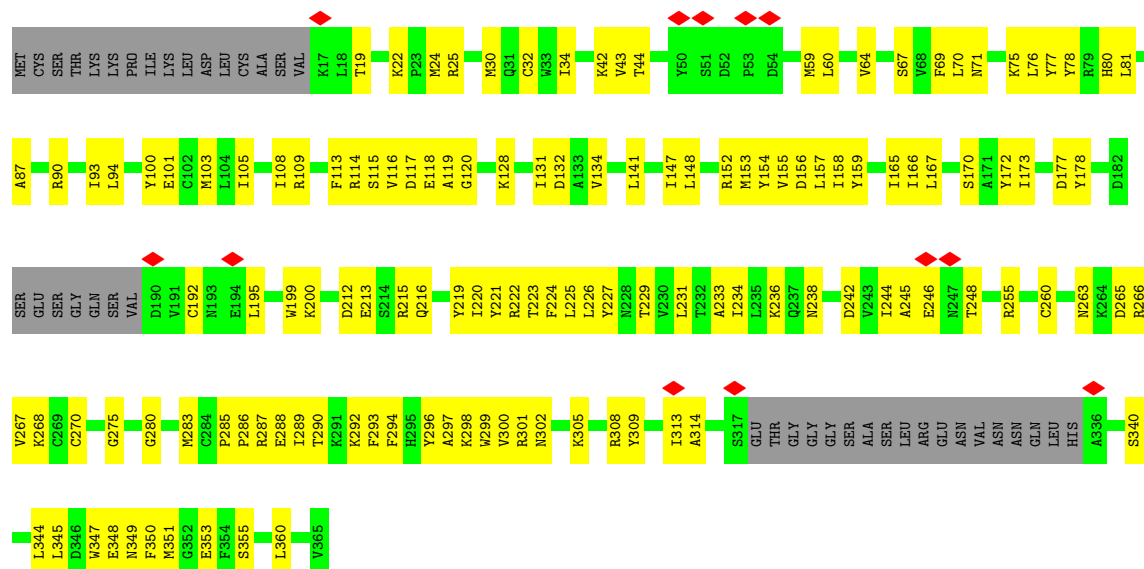
• Molecule 1: Protein AC54





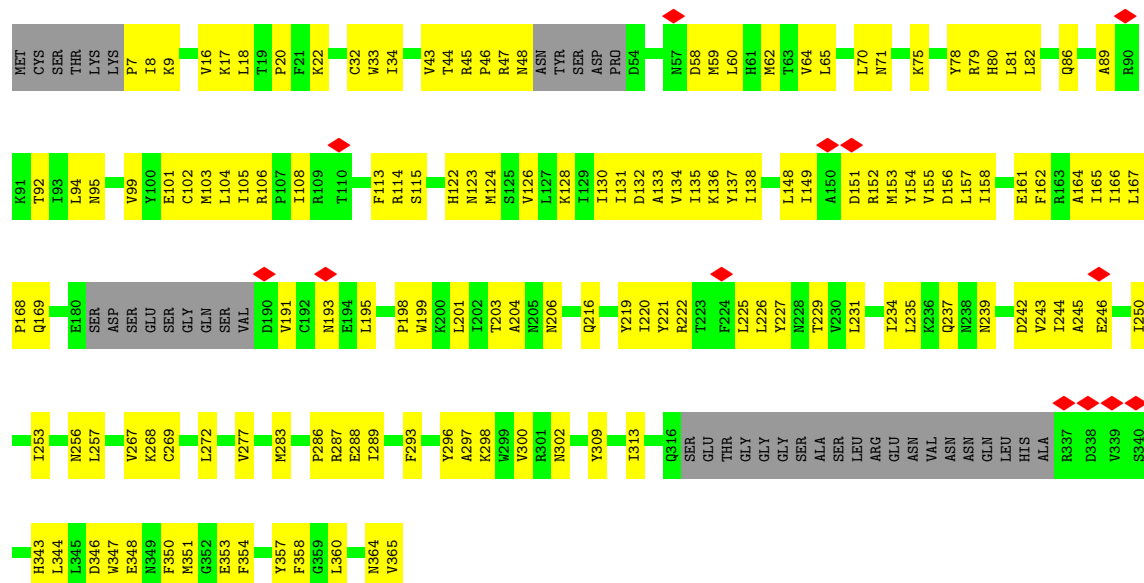
• Molecule 1: Protein AC54

Chain C: 52% 37% 11%

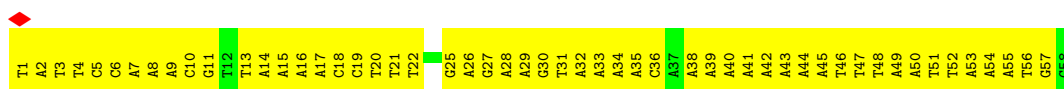


• Molecule 1: Protein AC54

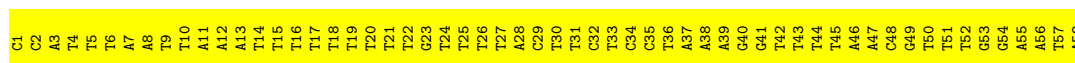
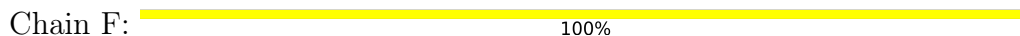
Chain D: 50% 39% 11%



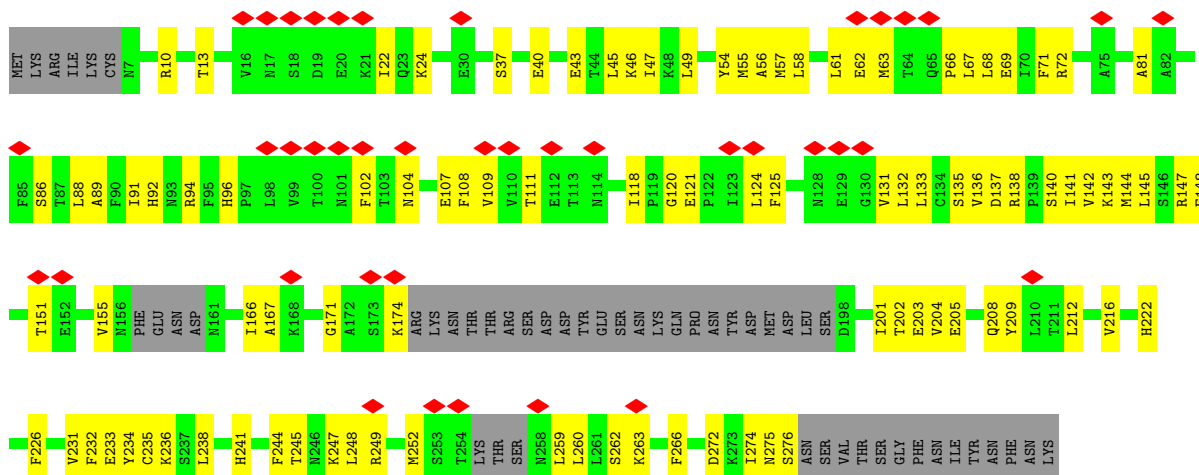
• Molecule 2: DNA (58-MER)



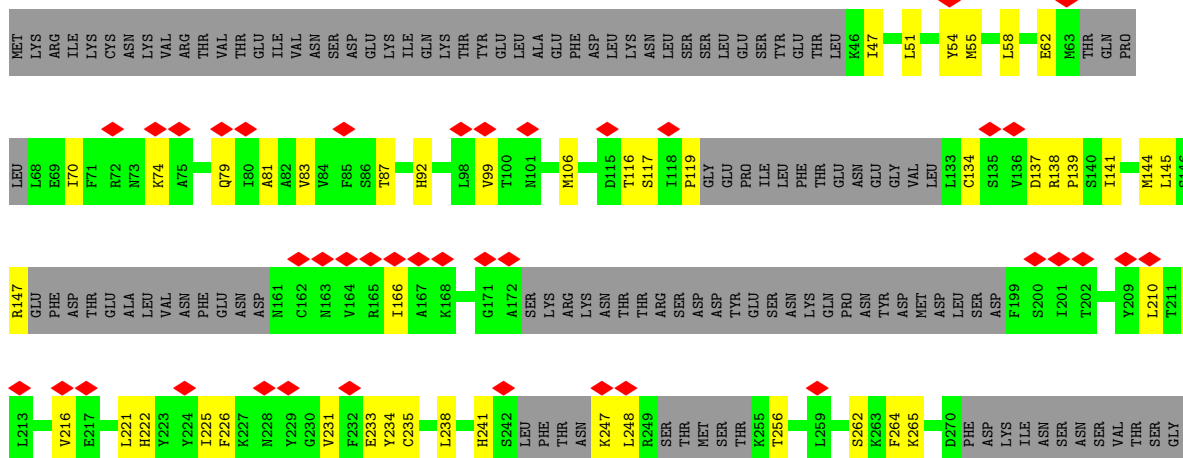
- Molecule 3: DNA (58-MER)



- Molecule 4: Occlusion-derived virus envelope protein E27



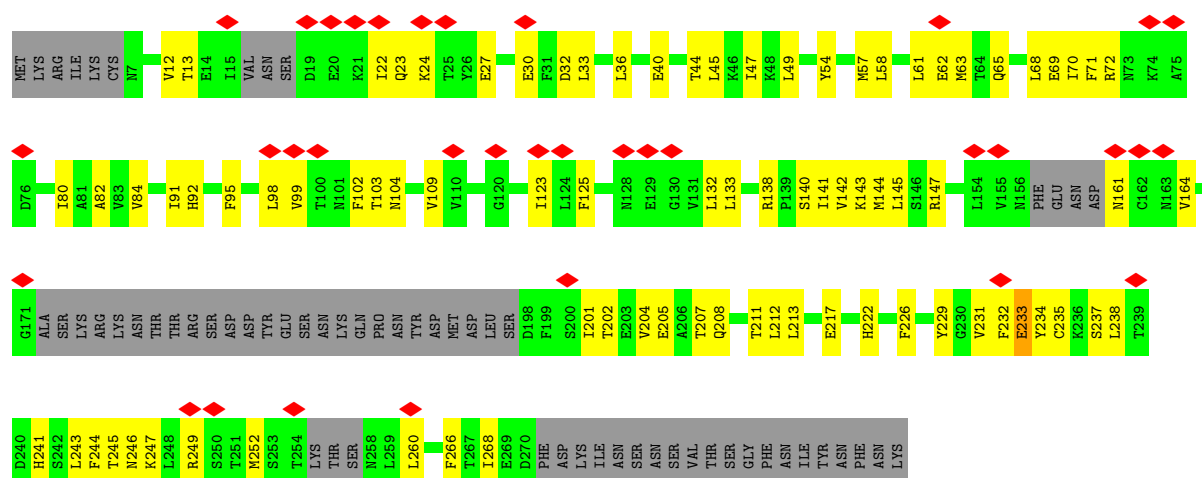
- Molecule 4: Occlusion-derived virus envelope protein E27



PHE
ASN
ILE
TYR
ASN
PHE
ASN
LYS

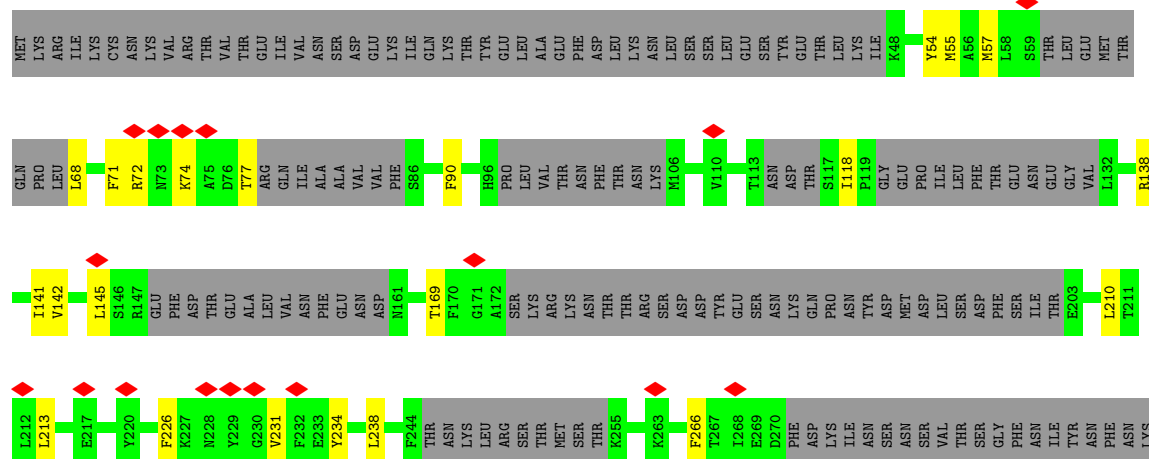
• Molecule 4: Occlusion-derived virus envelope protein E27

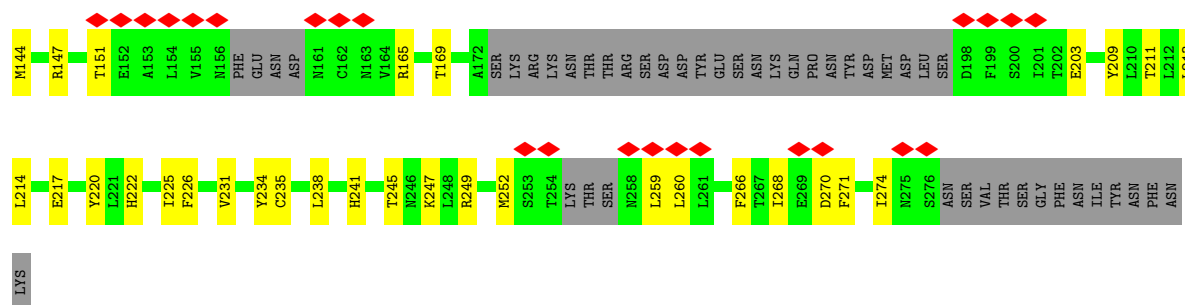
Chain K: 12% 50% 29% 21%



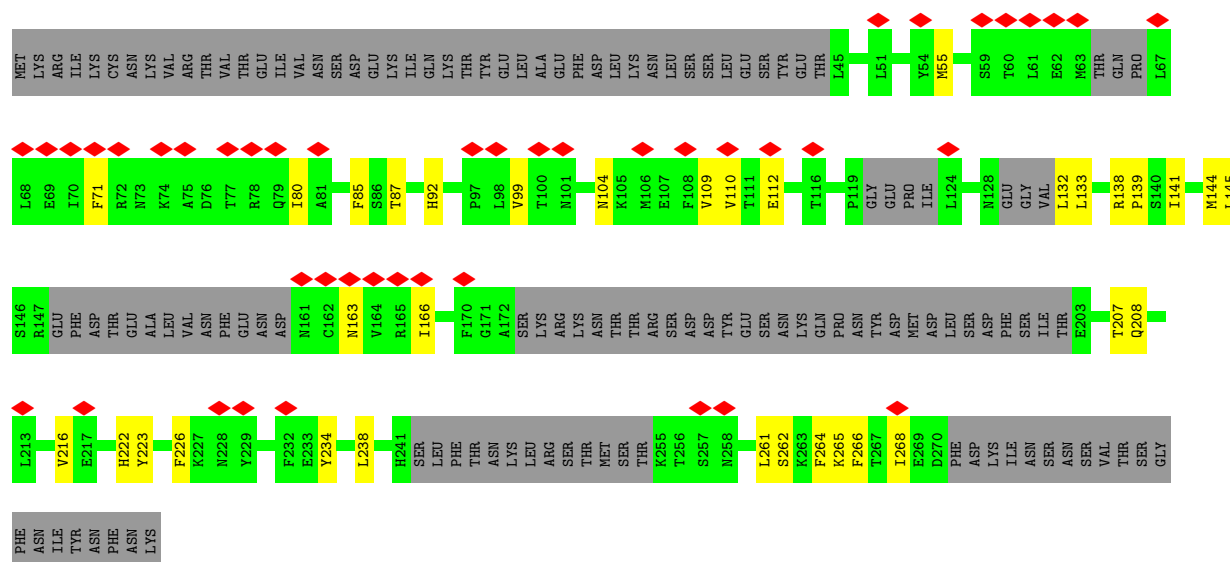
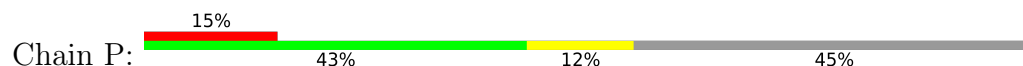
• Molecule 4: Occlusion-derived virus envelope protein E27

Chain L: 6% 37% 8% 55%

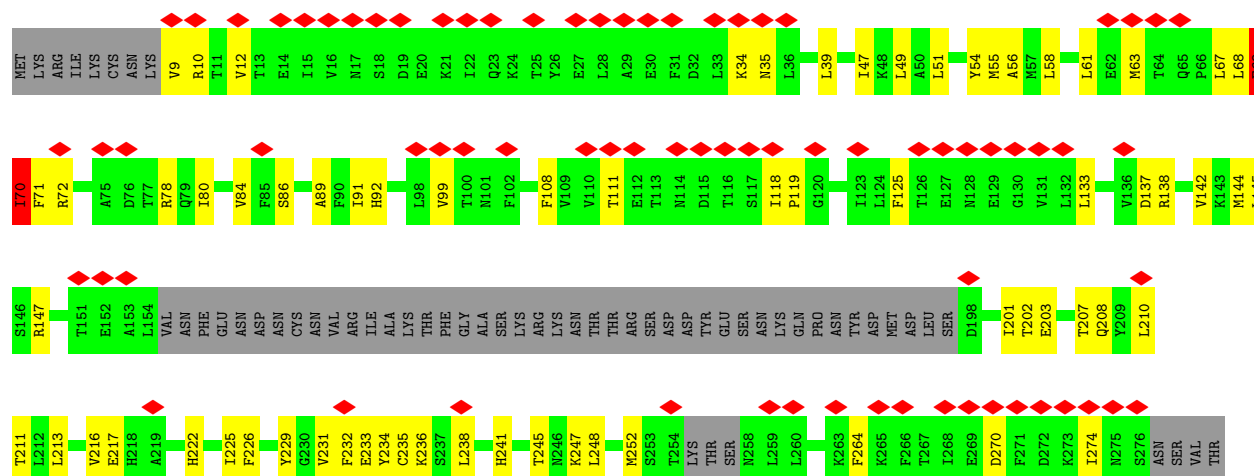




• Molecule 4: Occlusion-derived virus envelope protein E27

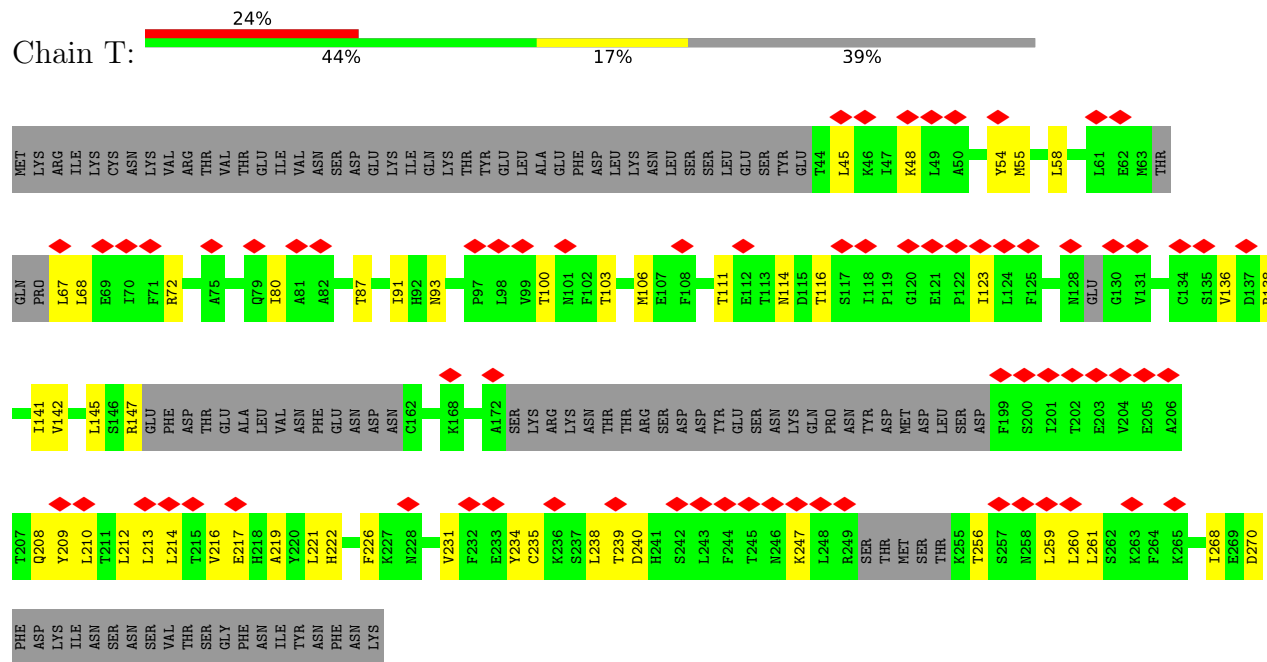


• Molecule 4: Occlusion-derived virus envelope protein E27

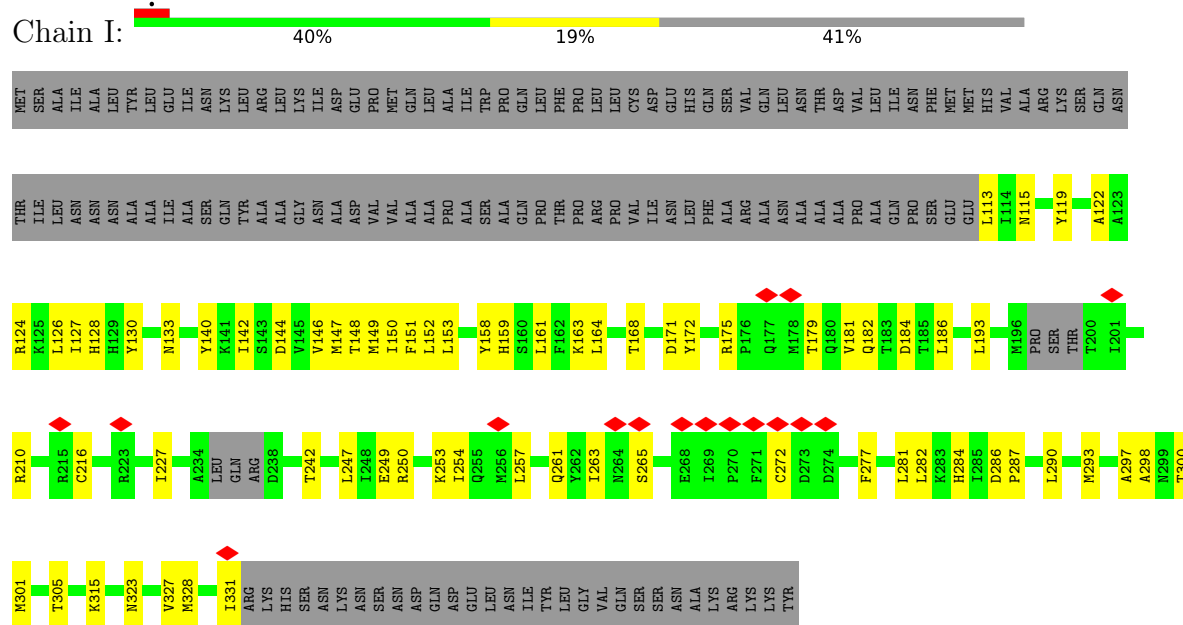


SER
GLY
PHE
ASN
ILE
TYR
ASN
PHE
ASN
LYS

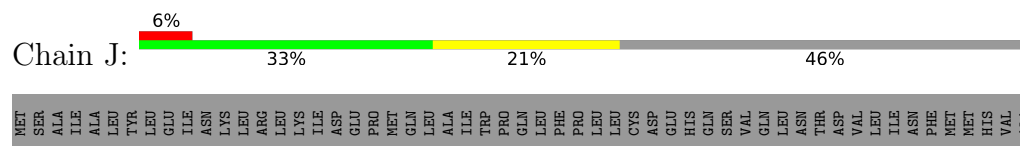
• Molecule 4: Occlusion-derived virus envelope protein E27

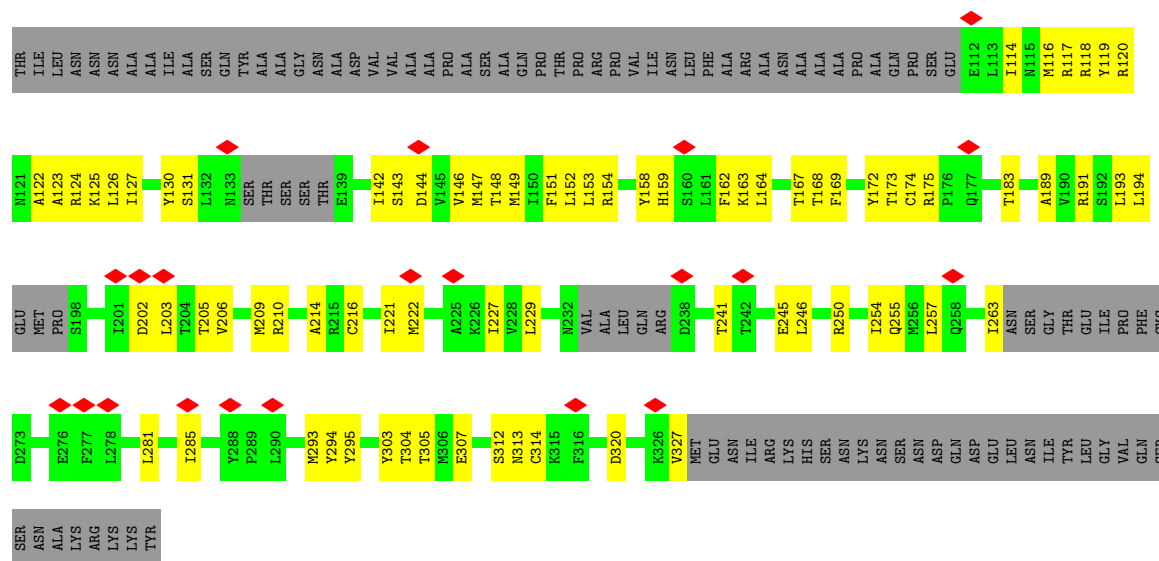


• Molecule 5: Protein C42



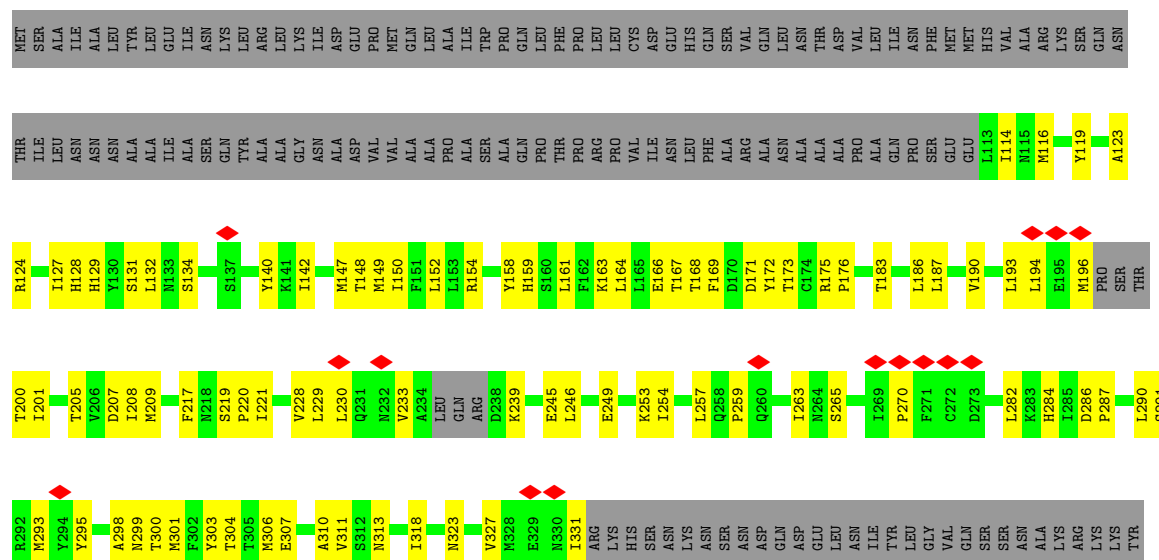
• Molecule 5: Protein C42





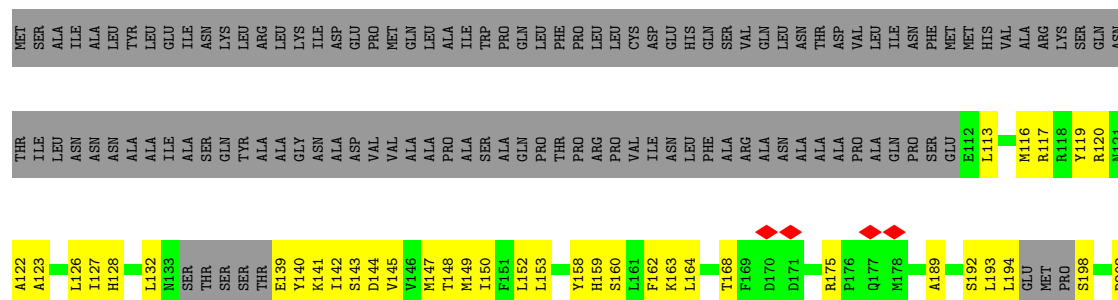
• Molecule 5: Protein C42

Chain M: 35% 24% 41%

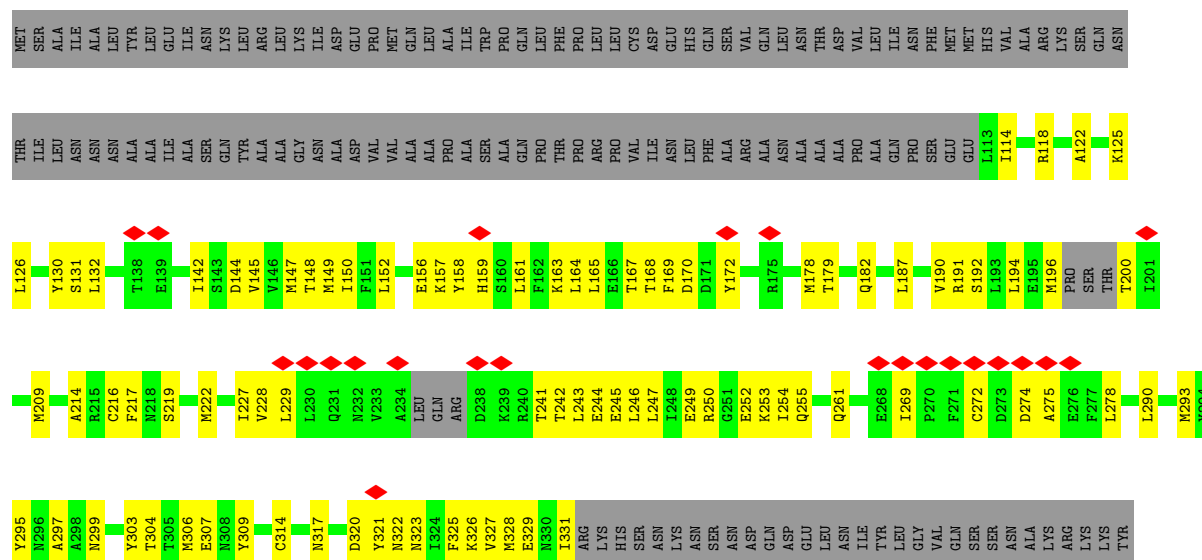


• Molecule 5: Protein C42

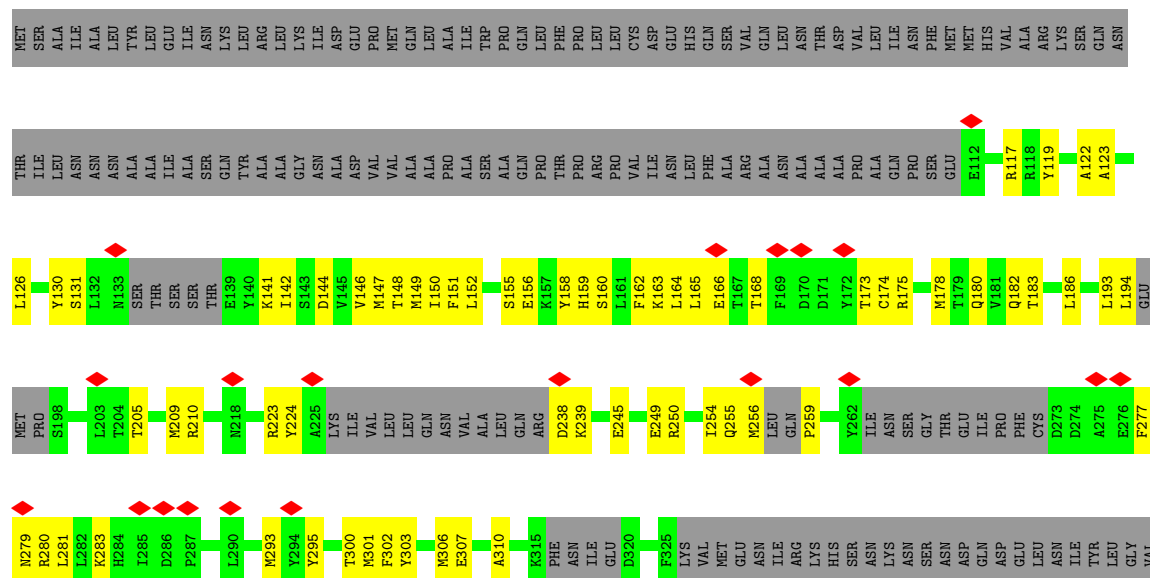
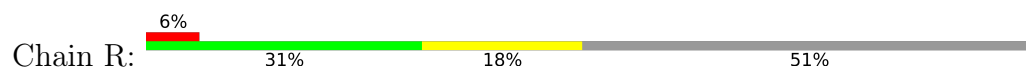
Chain N: 6% 33% 17% 50%



- Molecule 5: Protein C42



- Molecule 5: Protein C42



GLN
SER
SER
SER
ALA
LYS
LYS
ARG
LYS
TYR

● Molecule 5: Protein C42



MET
SER
ALA
ILE
ASN
LEU
TYR
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GLU
ILE
ASN
LYS
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ASP
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PRO
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TRP
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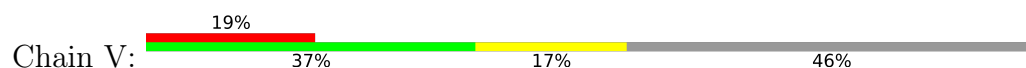
THR
ILE
ASN
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ALA
ALA
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SER
GLN
TYR
ALA
ALA
GLY
ASN
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LYS
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R124
H128
S131
L132
T135
S136
S137
E139
Y140
K141
I142
S143
D144
V145
V146
M147
T148
M149
I150
F151
L152
L153
Y158
H159
S160
L161
F162
K163
L164
L165
T168
F169
D170
D171
Y172
T173
C174
R175
P176
T183
A189
L193
L194
E195
M196
PRO
SER
THR
T200
L203

M209
R210
A214
S219
P220
I221
M222
Y224
A225
K226
I227
V228
L229
L230
A234
LEU
GLN
ARG
D238
K239
R240
L243
E244
E245
L246
E249
R250
G251
E252
K253
Q254
Q255
P259
Q260
Q261
Y262
L263
N264
S265
E268
I269
P270
F271
C272
D273
E277
L278
N279
R280
L281

ASN
ALA
LYS
ARG
LYS
LYS
TYR

● Molecule 5: Protein C42



MET
SER
ALA
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ASN
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TYR
LEU
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ARG
LEU
ASP
GLU
PRO
MET
GLN
LEU
ALA
ILE
TRP
PRO
GLN
PHE
PRO
LEU
LEU
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CYS
ASP
GLU
HIS
GLN
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GLN
ASN

L132
M133
S134
T135
S136
S137
T138
I142
S143
V145
V146
M147
T148
M149
I150
F151
L152
L153
K157
Y158
L161
F162
K163
L164
L165
E166
T167
T168
F169
D170
P176
GLN
MET
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L187
D188
A189
V190
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GLU
MET
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S198
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T200
I201
D202
L203
T204
T205
V206

R210
F213
A214
F217
I221
A225
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I227
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R250
G251
E252
K253
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Q255
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P259
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I263
ASN
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GLY
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PHE
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D273
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E276
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M279
R280
L281
L282
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E307
V311
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F316
N317
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D320
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I324
F325
K326
V327
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ASP
LEU
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ASN
ILE
TYR
LEU
GLY
VAL

GLN
SER
SER
SER
ALA
LYS
ARG
LYS
LYS
TYR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12477	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.15	0/2783	0.37	0/3772
1	B	0.16	0/2823	0.37	0/3825
1	C	0.16	0/2724	0.41	0/3691
1	D	0.17	0/2728	0.42	0/3693
2	E	0.19	0/1350	0.34	0/2081
3	F	0.19	0/1313	0.40	0/2025
4	G	0.14	0/1973	0.34	0/2664
4	H	0.13	0/1321	0.32	0/1774
4	K	0.16	0/1880	0.42	2/2538 (0.1%)
4	L	0.11	0/1076	0.25	0/1439
4	O	0.15	0/1958	0.37	0/2645
4	P	0.13	0/1322	0.31	0/1778
4	S	0.17	0/1837	0.40	2/2484 (0.1%)
4	T	0.12	0/1464	0.29	0/1972
5	I	0.14	0/1790	0.35	0/2415
5	J	0.16	0/1648	0.36	0/2219
5	M	0.16	0/1790	0.38	0/2415
5	N	0.14	0/1539	0.37	0/2065
5	Q	0.17	0/1790	0.40	0/2415
5	R	0.14	0/1511	0.36	0/2030
5	U	0.16	0/1790	0.35	0/2415
5	V	0.12	0/1656	0.30	0/2231
All	All	0.15	0/40066	0.37	4/54586 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	233	GLU	CA-C-N	-5.48	112.51	120.29
4	K	233	GLU	C-N-CA	-5.48	112.51	120.29
4	S	69	GLU	N-CA-C	-5.43	106.49	113.23
4	S	70	ILE	N-CA-C	-5.34	104.20	111.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2717	0	2673	112	0
1	B	2757	0	2724	139	0
1	C	2660	0	2624	124	0
1	D	2666	0	2655	135	0
2	E	1198	0	654	113	0
3	F	1177	0	670	156	0
4	G	1941	0	1954	114	0
4	H	1301	0	1330	46	0
4	K	1850	0	1862	84	0
4	L	1061	0	1072	20	0
4	O	1926	0	1936	86	0
4	P	1302	0	1328	27	0
4	S	1805	0	1811	72	0
4	T	1440	0	1476	46	0
5	I	1760	0	1756	74	0
5	J	1622	0	1623	89	0
5	M	1760	0	1756	84	0
5	N	1517	0	1507	65	0
5	Q	1760	0	1756	89	0
5	R	1488	0	1469	74	0
5	U	1760	0	1756	92	0
5	V	1630	0	1628	65	0
All	All	39098	0	38020	1633	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 21.

The worst 5 of 1633 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)
4:K:47:ILE:HD12	4:K:260:LEU:HD12	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ILE:HD11	1:C:313:ILE:HG21	1.43	0.96
5:V:152:LEU:HD12	5:V:161:LEU:HD11	1.57	0.85
4:G:248:LEU:HD12	4:G:252:MET:HB2	1.59	0.85
4:O:54:TYR:OH	4:O:87:THR:HG22	1.78	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	328/365 (90%)	296 (90%)	32 (10%)	0	100	100
1	B	331/365 (91%)	305 (92%)	26 (8%)	0	100	100
1	C	318/365 (87%)	283 (89%)	35 (11%)	0	100	100
1	D	317/365 (87%)	286 (90%)	31 (10%)	0	100	100
4	G	232/290 (80%)	219 (94%)	13 (6%)	0	100	100
4	H	146/290 (50%)	141 (97%)	5 (3%)	0	100	100
4	K	218/290 (75%)	206 (94%)	12 (6%)	0	100	100
4	L	112/290 (39%)	111 (99%)	1 (1%)	0	100	100
4	O	230/290 (79%)	216 (94%)	14 (6%)	0	100	100
4	P	146/290 (50%)	140 (96%)	6 (4%)	0	100	100
4	S	216/290 (74%)	204 (94%)	12 (6%)	0	100	100
4	T	166/290 (57%)	161 (97%)	4 (2%)	1 (1%)	22	61
5	I	207/361 (57%)	196 (95%)	11 (5%)	0	100	100
5	J	184/361 (51%)	172 (94%)	12 (6%)	0	100	100
5	M	207/361 (57%)	194 (94%)	13 (6%)	0	100	100
5	N	165/361 (46%)	159 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Q	207/361 (57%)	195 (94%)	12 (6%)	0	100	100
5	R	164/361 (45%)	156 (95%)	8 (5%)	0	100	100
5	U	207/361 (57%)	194 (94%)	13 (6%)	0	100	100
5	V	186/361 (52%)	174 (94%)	12 (6%)	0	100	100
All	All	4287/6668 (64%)	4008 (94%)	278 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	T	247	LYS

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	303/331 (92%)	303 (100%)	0	100	100
1	B	308/331 (93%)	308 (100%)	0	100	100
1	C	296/331 (89%)	296 (100%)	0	100	100
1	D	297/331 (90%)	297 (100%)	0	100	100
4	G	224/273 (82%)	224 (100%)	0	100	100
4	H	148/273 (54%)	148 (100%)	0	100	100
4	K	213/273 (78%)	213 (100%)	0	100	100
4	L	120/273 (44%)	120 (100%)	0	100	100
4	O	222/273 (81%)	222 (100%)	0	100	100
4	P	148/273 (54%)	148 (100%)	0	100	100
4	S	209/273 (77%)	207 (99%)	2 (1%)	73	82
4	T	164/273 (60%)	164 (100%)	0	100	100
5	I	201/326 (62%)	201 (100%)	0	100	100
5	J	184/326 (56%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	201/326 (62%)	201 (100%)	0	100	100
5	N	171/326 (52%)	171 (100%)	0	100	100
5	Q	201/326 (62%)	201 (100%)	0	100	100
5	R	168/326 (52%)	168 (100%)	0	100	100
5	U	201/326 (62%)	201 (100%)	0	100	100
5	V	186/326 (57%)	186 (100%)	0	100	100
All	All	4165/6116 (68%)	4163 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	S	69	GLU
4	S	70	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
5	N	159	HIS
5	R	129	HIS
4	O	92	HIS
4	O	258	ASN
4	T	93	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

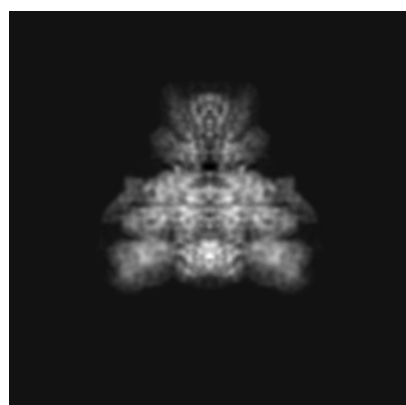
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51803. These allow visual inspection of the internal detail of the map and identification of artifacts.

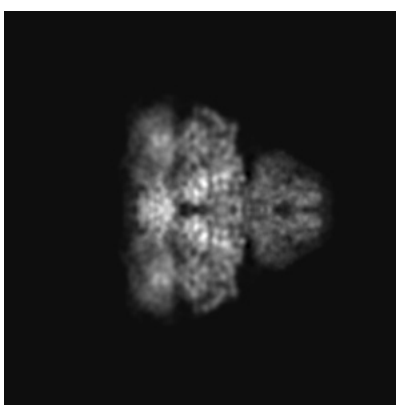
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

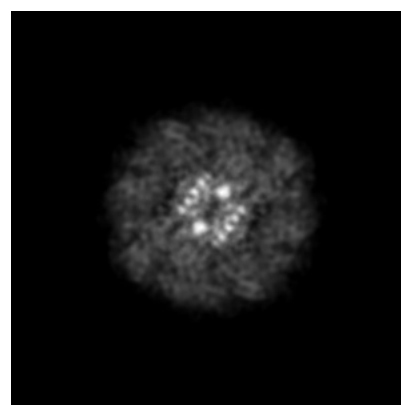
6.1.1 Primary map



X



Y

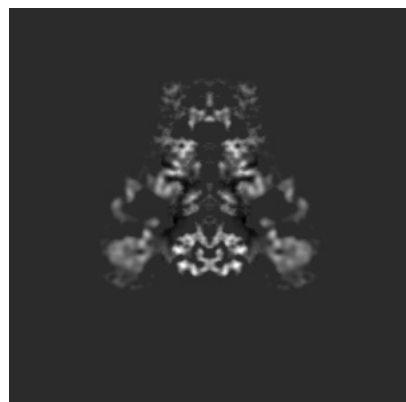


Z

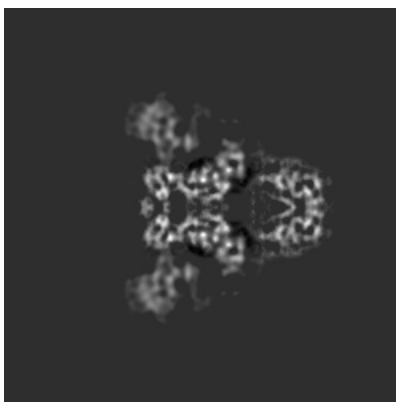
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

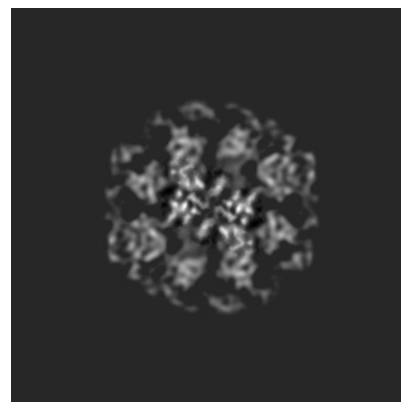
6.2.1 Primary map



X Index: 150



Y Index: 150

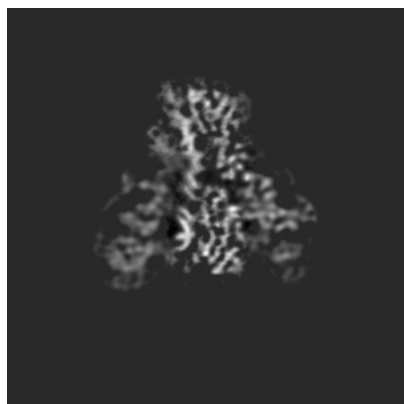


Z Index: 150

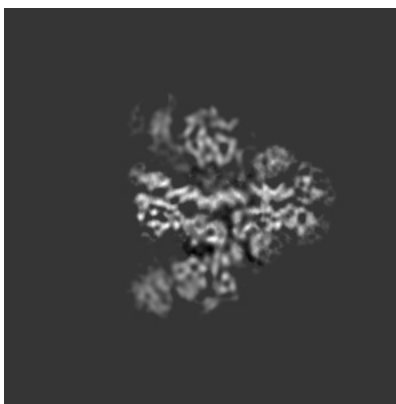
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

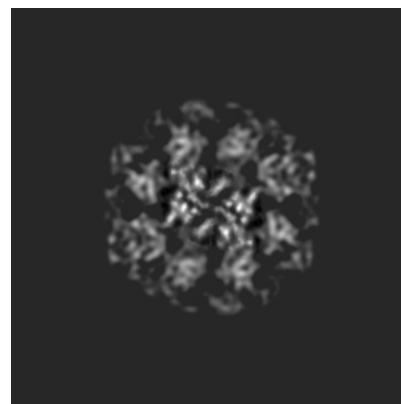
6.3.1 Primary map



X Index: 139



Y Index: 164

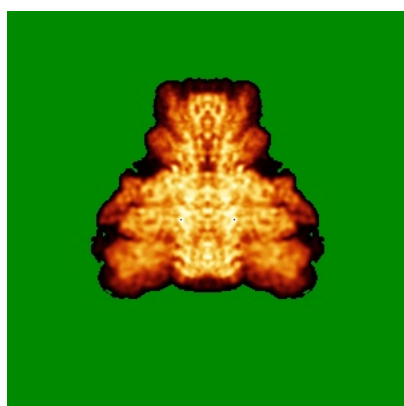


Z Index: 149

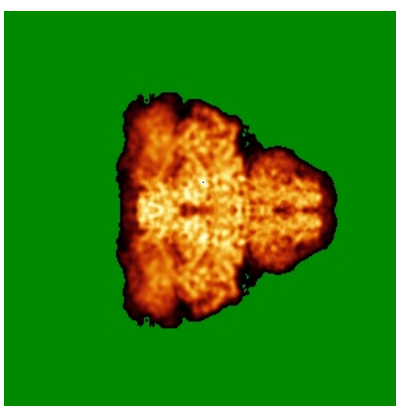
The images above show the largest variance slices of the map in three orthogonal directions.

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

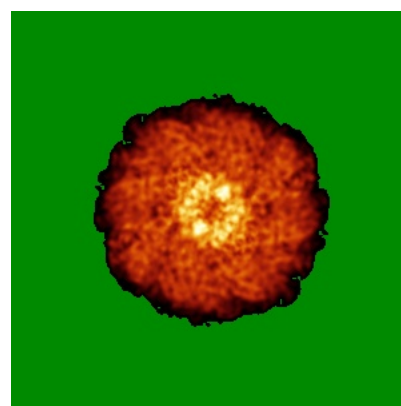
6.4.1 Primary map



X



Y

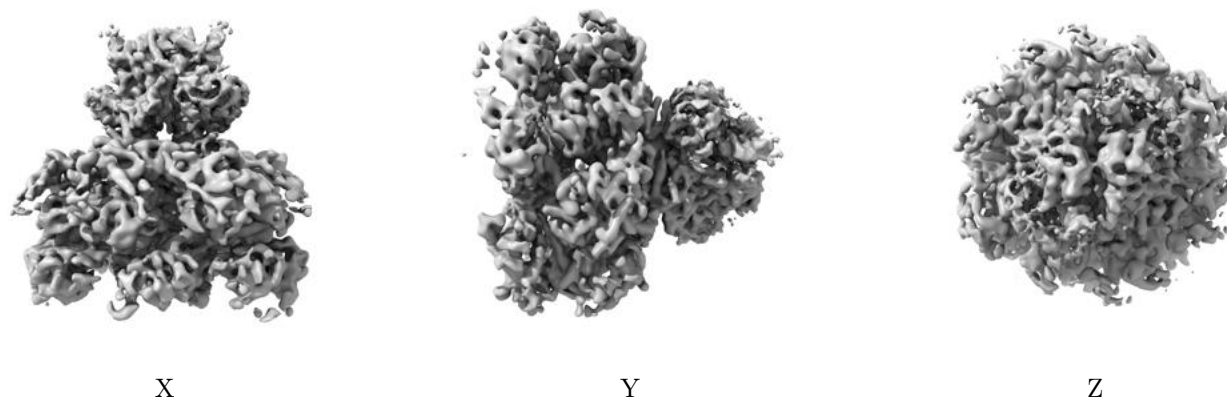


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

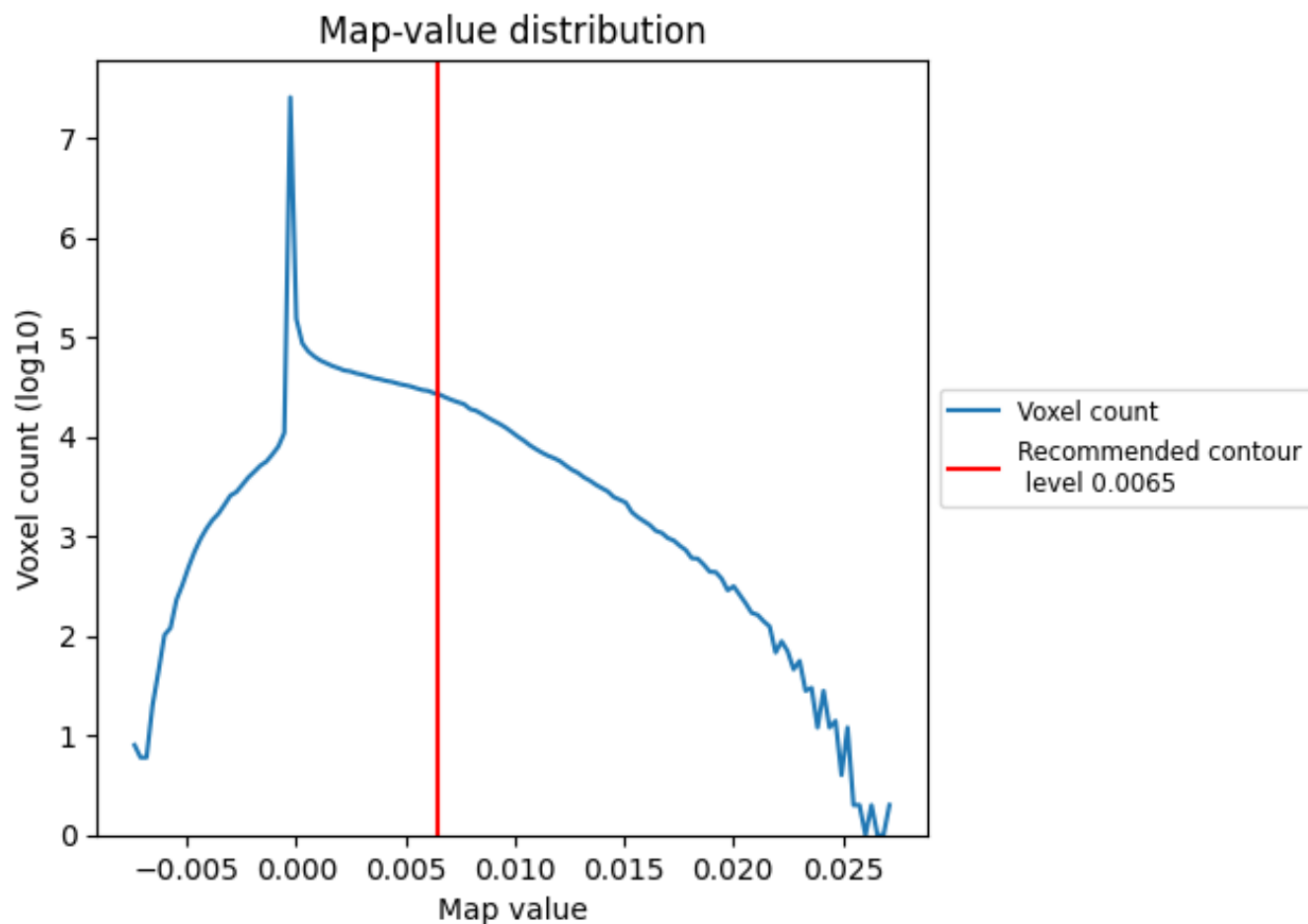
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

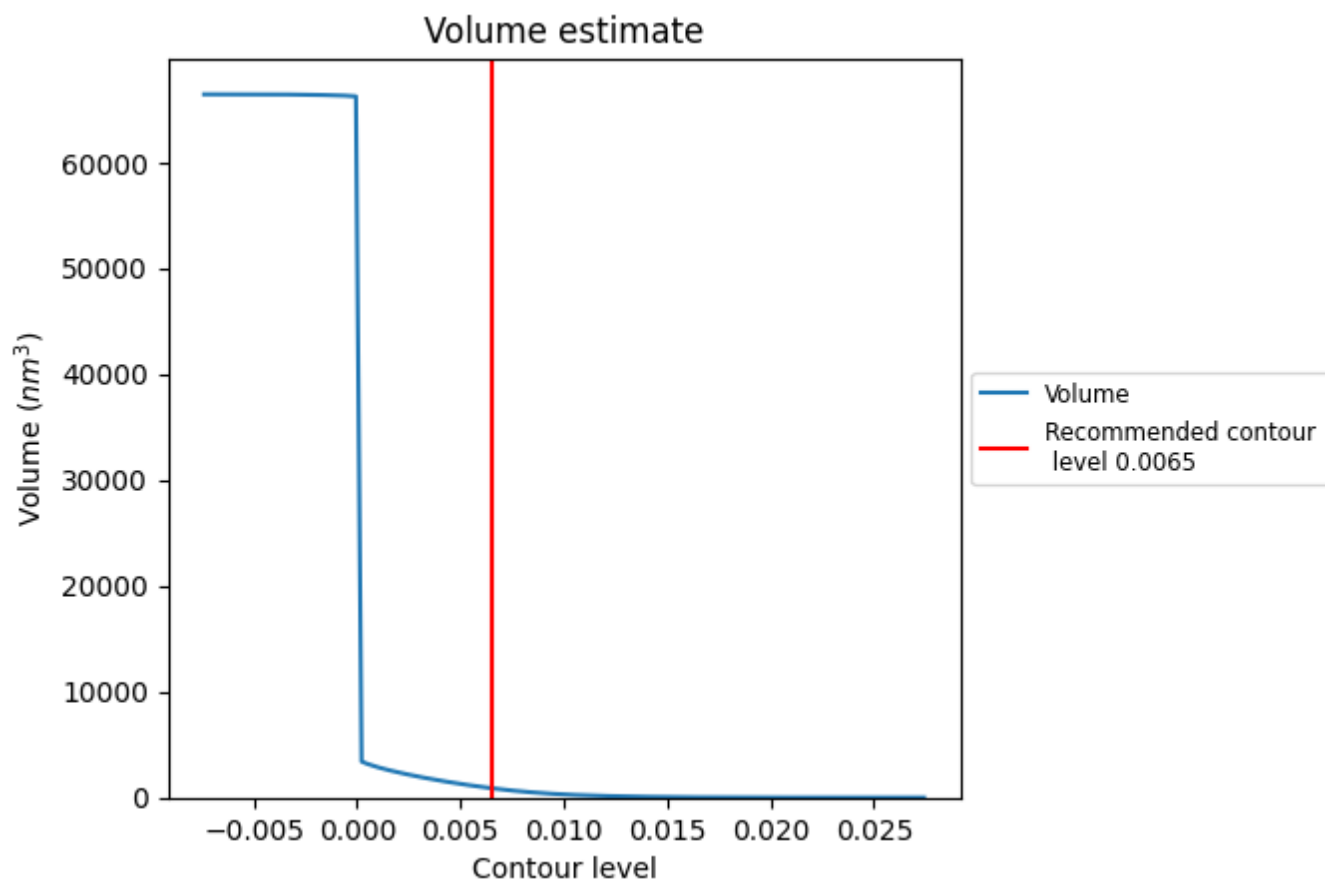
This section contains the results of statistical analysis of the map.

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.

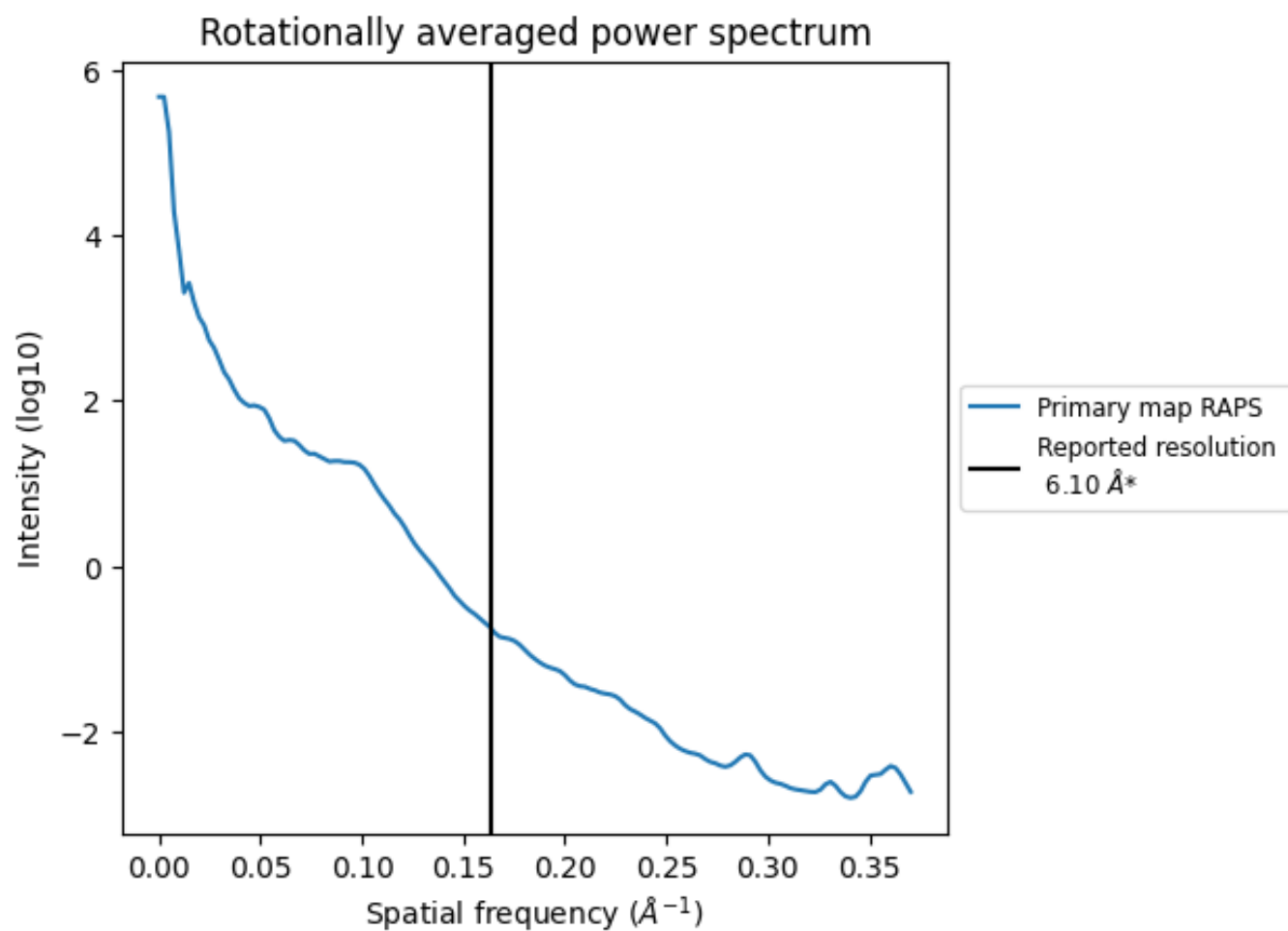
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 886 nm³; this corresponds to an approximate mass of 800 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 0.164 Å⁻¹

8 Fourier-Shell correlation

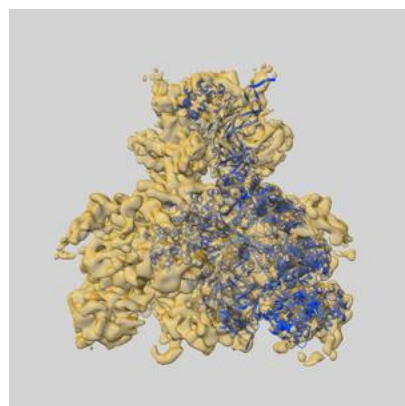
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

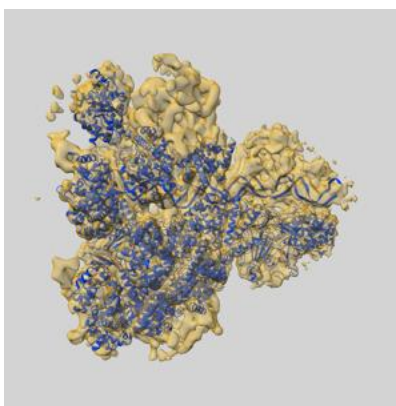
This section contains information regarding the fit between EMDB map EMD-51803 and PDB model 9H2H. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

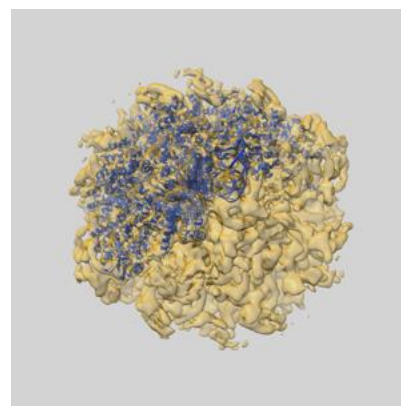
9.1.1 Map-model overlay [i](#)



X

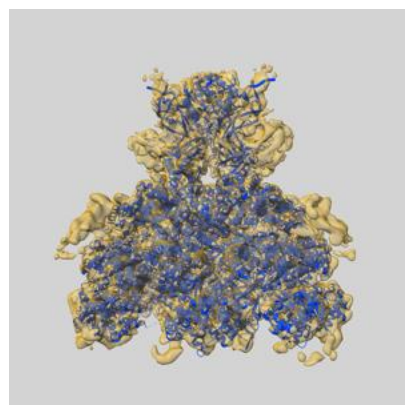


Y

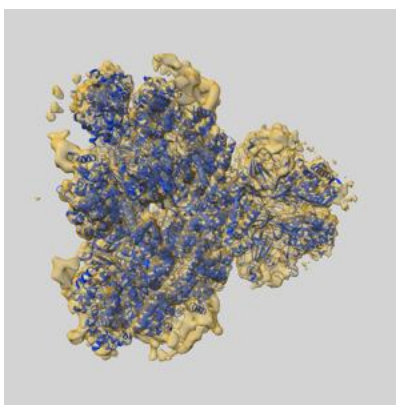


Z

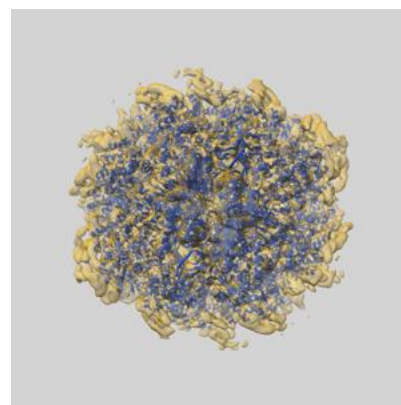
9.1.2 Map-model assembly overlay [i](#)



X



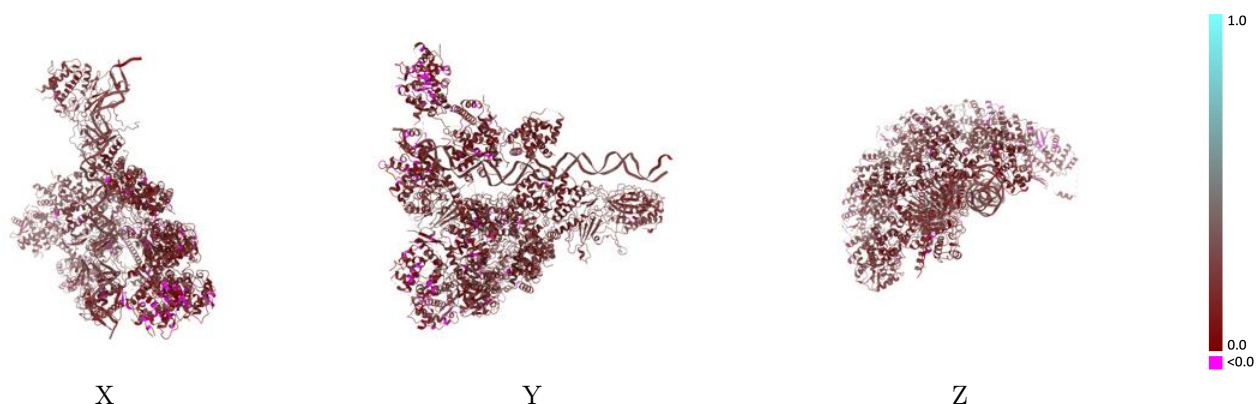
Y



Z

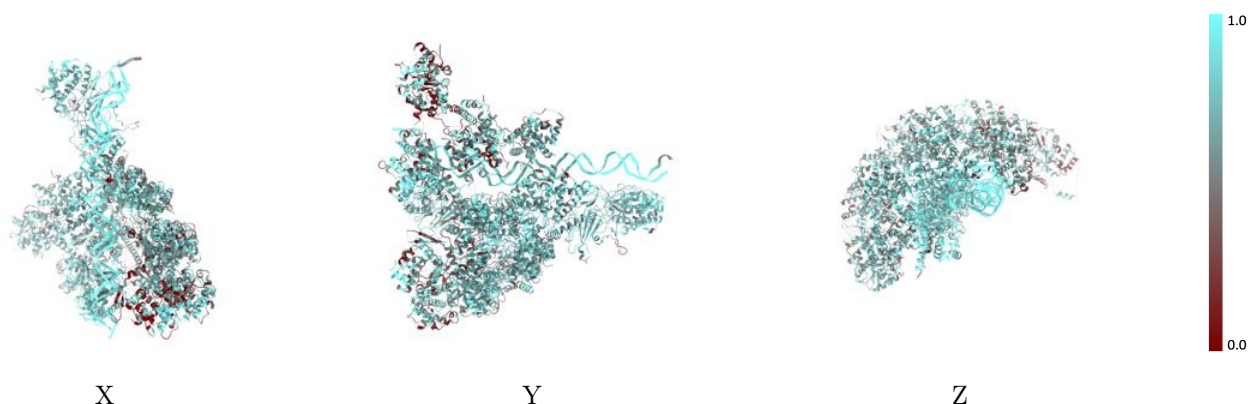
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



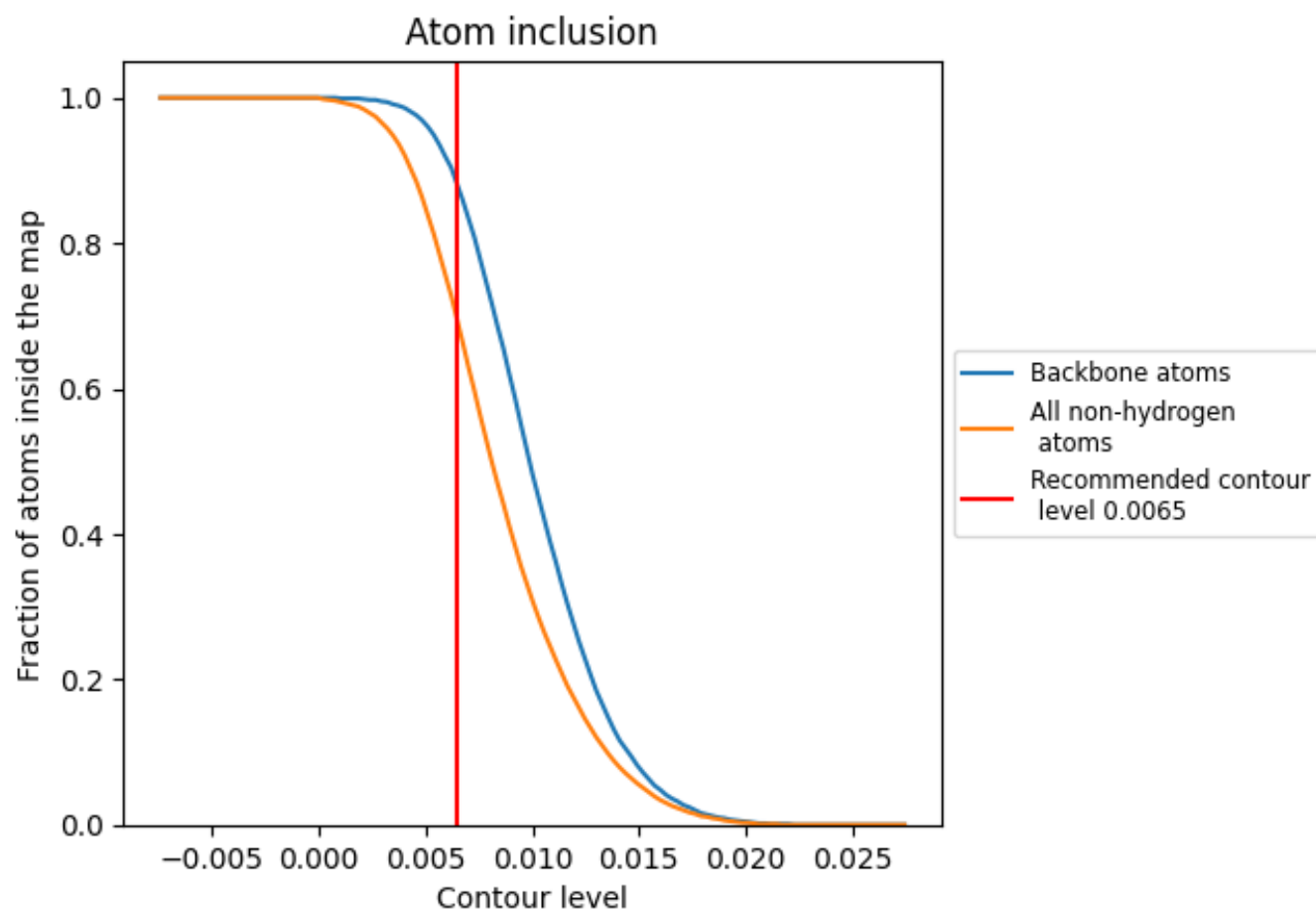
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0065).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 69% 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 (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.1920
A	 0.7500	 0.2170
B	 0.7680	 0.2250
C	 0.7900	 0.2300
D	 0.7850	 0.2170
E	 0.9240	 0.2670
F	 0.9520	 0.2780
G	 0.6420	 0.1770
H	 0.6240	 0.1580
I	 0.7220	 0.1970
J	 0.7100	 0.1790
K	 0.6480	 0.1760
L	 0.7210	 0.1580
M	 0.7060	 0.1870
N	 0.7010	 0.1780
O	 0.5770	 0.1710
P	 0.6370	 0.1540
Q	 0.6640	 0.1880
R	 0.6730	 0.1840
S	 0.4990	 0.1580
T	 0.5360	 0.1260
U	 0.6310	 0.1760
V	 0.5370	 0.1650

