



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:09 PM UTC

PDB ID : 6BT3 / pdb_00006bt3
EMDB ID : EMD-8243
Title : High-Resolution Structure Analysis of Antibody V5 Conformational Epitope on Human Papillomavirus 16
Authors : Guan, J.; Bywaters, S.M.; Brendle, S.A.; Ashley, R.E.; Makhov, A.M.; Conway, J.F.; Christensen, N.D.; Hafenstein, S.
Deposited on : 2017-12-05
Resolution : 4.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

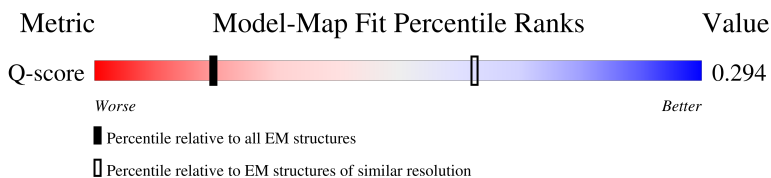
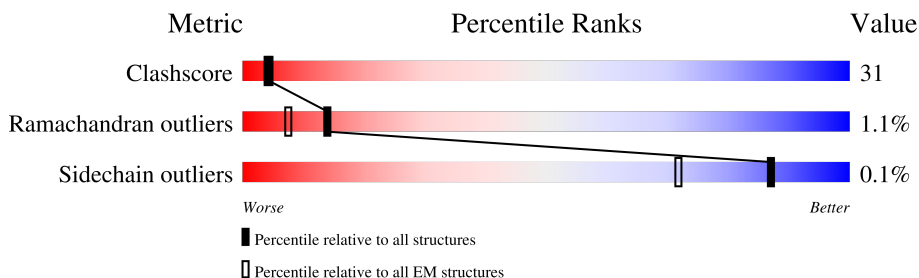
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



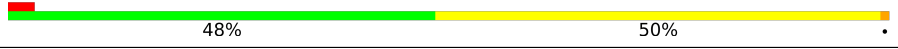
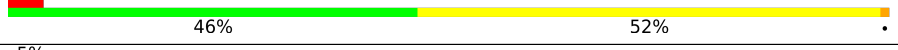
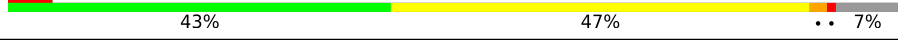
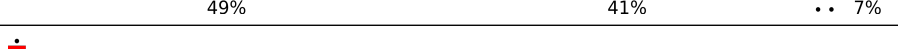
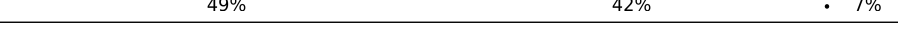
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	220	 46% 53% .
1	C	220	 46% 53% .
1	E	220	 50% 49% .
1	G	220	 47% 51% .

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Mol	Chain	Length	Quality of chain
2	B	223	 47% 52%
2	D	223	 47% 52%
2	F	223	 48% 50%
2	H	223	 46% 52%
3	I	503	 43% 47% 5% 7%
3	J	503	 48% 42% 9%
3	K	503	 50% 41% 7%
3	L	503	 50% 41% 7%
3	M	503	 49% 41% 7%
3	N	503	 49% 42% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35383 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 V5 Fab Light-chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	0	0
			1673	1044	281	340	8		
1	C	220	Total	C	N	O	S	0	0
			1673	1044	281	340	8		
1	E	220	Total	C	N	O	S	0	0
			1673	1044	281	340	8		
1	G	220	Total	C	N	O	S	0	0
			1673	1044	281	340	8		

- Molecule 2 is a protein called V5 Fab Heavy-chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	223	Total	C	N	O	S	0	0
			1675	1071	268	330	6		
2	D	223	Total	C	N	O	S	0	0
			1675	1071	268	330	6		
2	F	223	Total	C	N	O	S	0	0
			1675	1071	268	330	6		
2	H	223	Total	C	N	O	S	0	0
			1675	1071	268	330	6		

- Molecule 3 is a protein called Major capsid protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	468	Total	C	N	O	S	0	0
			3675	2347	617	690	21		
3	J	460	Total	C	N	O	S	0	0
			3614	2304	609	680	21		
3	K	469	Total	C	N	O	S	0	0
			3686	2356	618	691	21		
3	L	468	Total	C	N	O	S	0	0
			3675	2347	617	690	21		
3	M	467	Total	C	N	O	S	0	0
			3666	2341	615	689	21		

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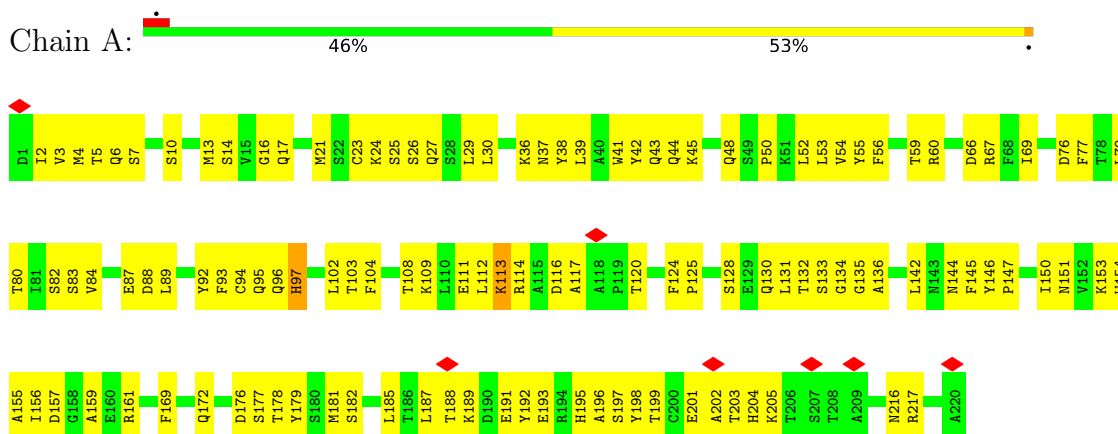
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	468	Total	C	N	O	S	0	0
			3675	2347	617	690	21		

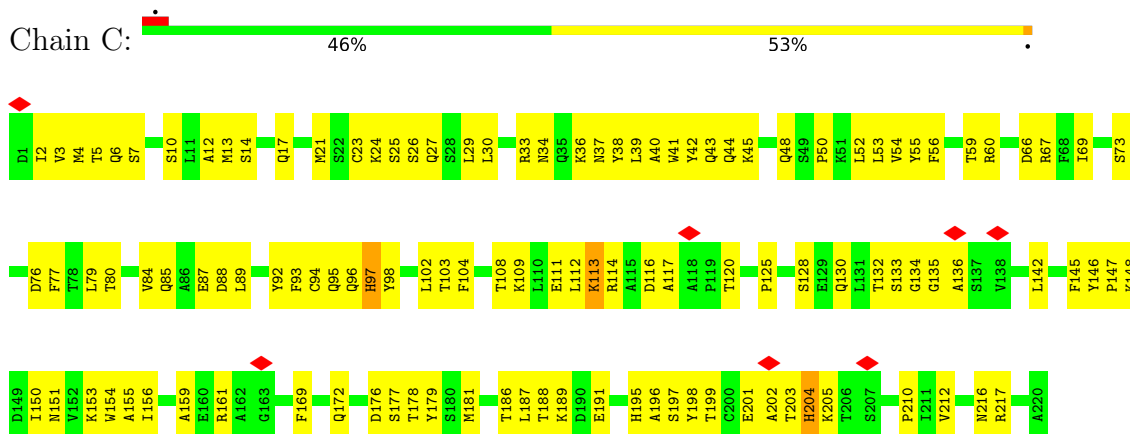
3 Residue-property plots

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.

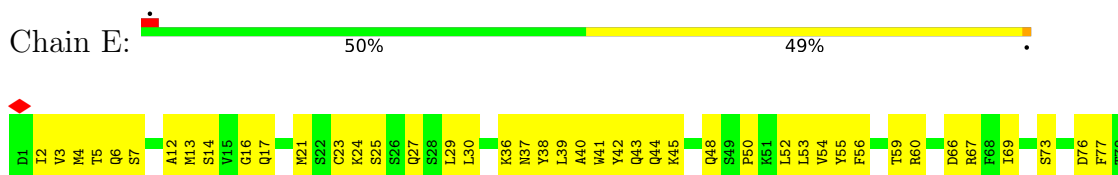
• Molecule 1: V5 Fab Light-chain

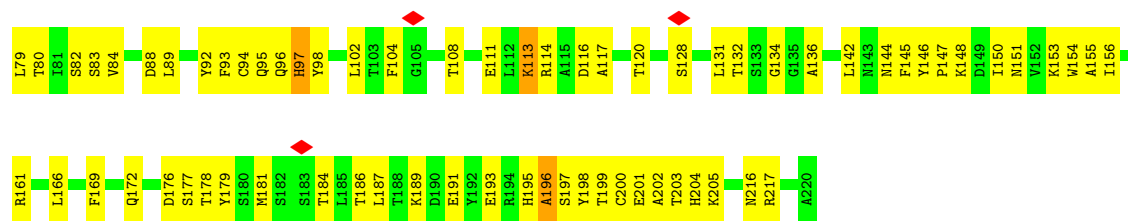


• Molecule 1: V5 Fab Light-chain

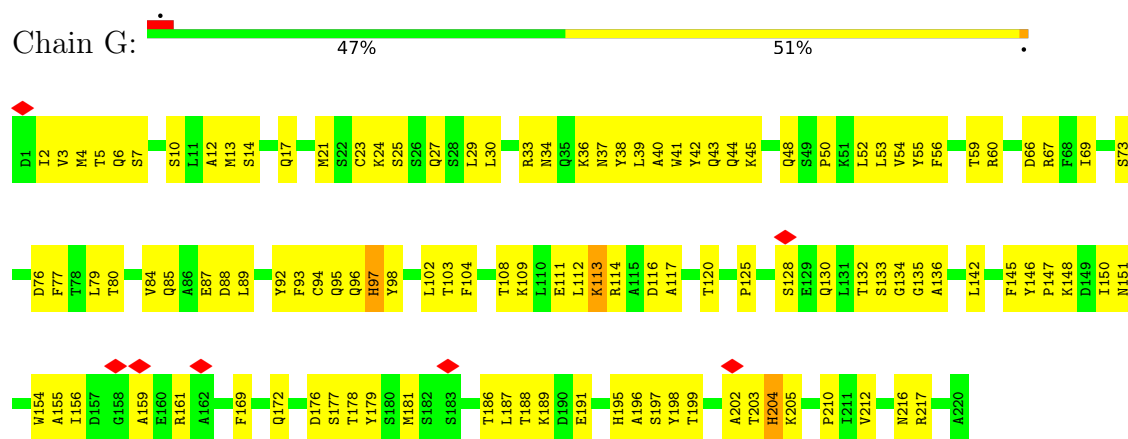


• Molecule 1: V5 Fab Light-chain

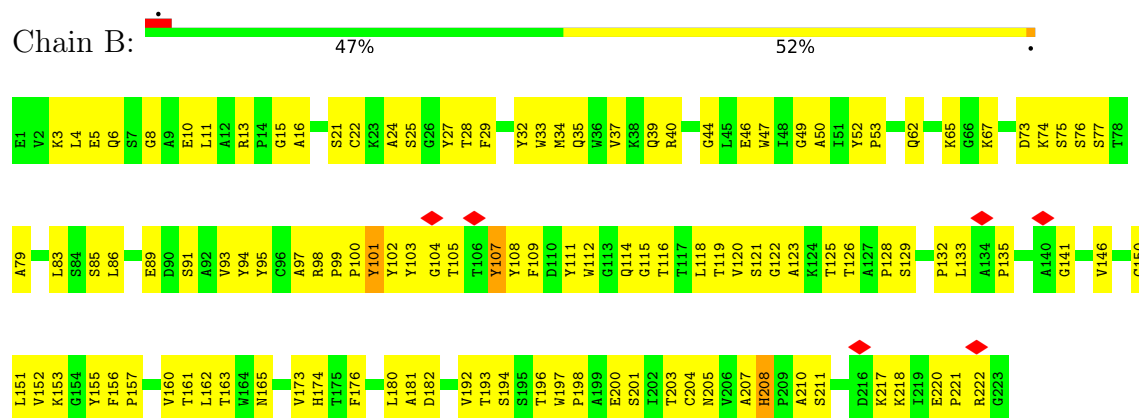




• Molecule 1: V5 Fab Light-chain



• Molecule 2: V5 Fab Heavy-chain

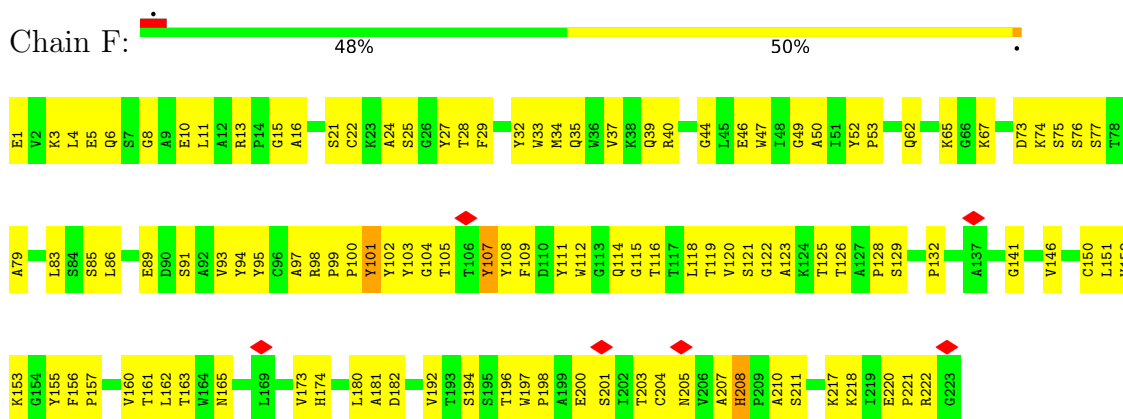


• Molecule 2: V5 Fab Heavy-chain



- Molecule 2: V5 Fab Heavy-chain

Chain F:



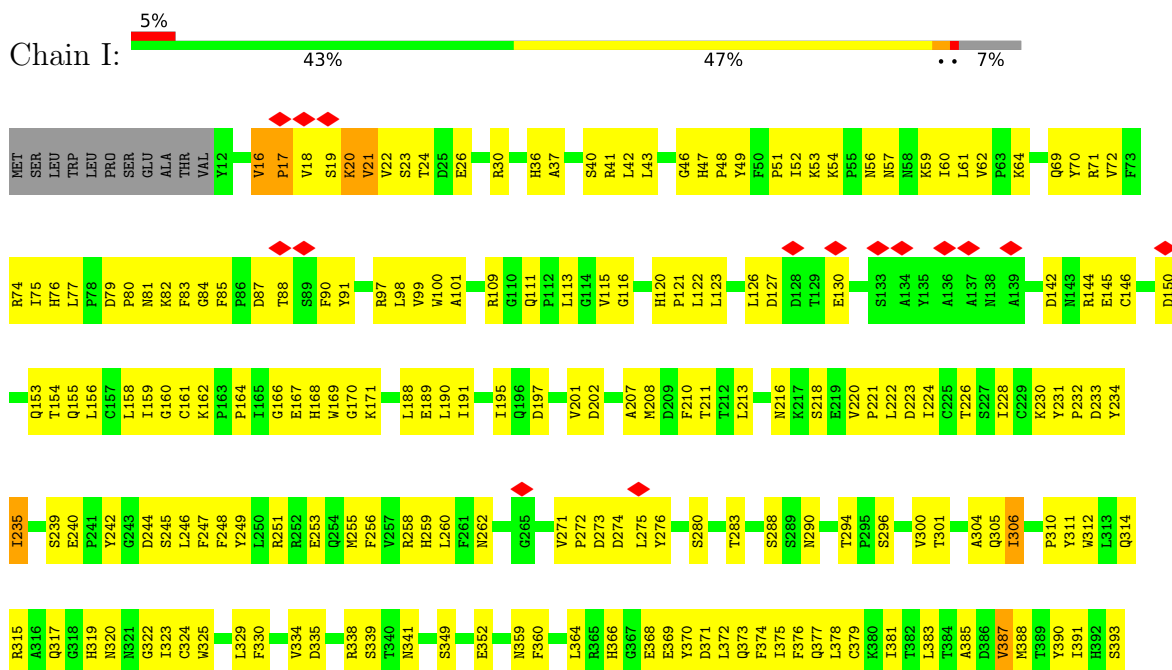
- Molecule 2: V5 Fab Heavy-chain

Chain H:



- Molecule 3: Major capsid protein L1

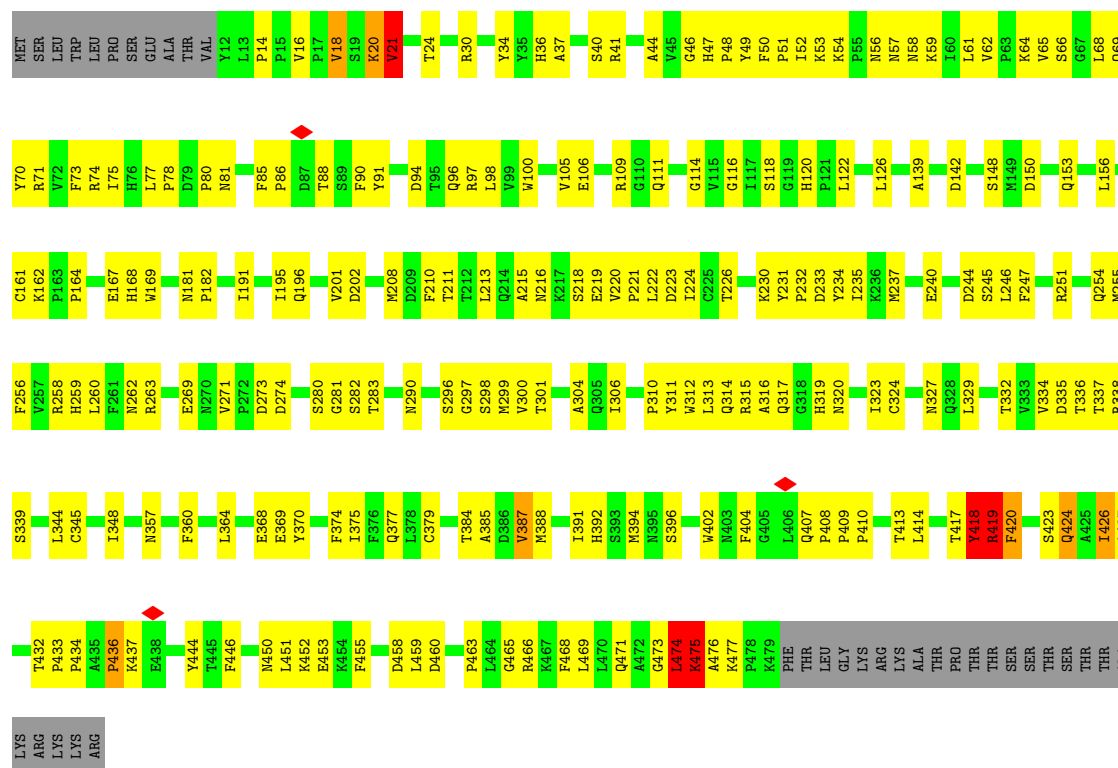
Chain I:



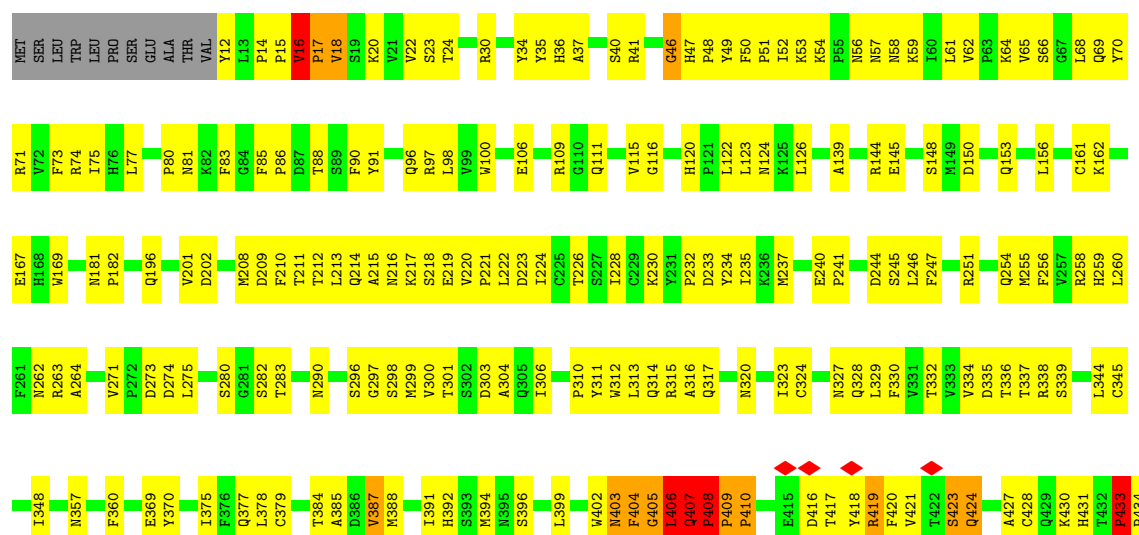




• Molecule 3: Major capsid protein L1



• Molecule 3: Major capsid protein L1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	19.469	Depositor
Minimum map value	-14.719	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	910.0, 910.0, 910.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.75, 1.75, 1.75	Depositor

5 Model quality

5.1 Standard geometry

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	0.46	3/1708 (0.2%)	0.54	2/2314 (0.1%)
1	C	0.46	3/1708 (0.2%)	0.54	2/2314 (0.1%)
1	E	0.46	3/1708 (0.2%)	0.55	2/2314 (0.1%)
1	G	0.46	3/1708 (0.2%)	0.54	2/2314 (0.1%)
2	B	0.44	2/1725 (0.1%)	0.57	0/2358
2	D	0.43	2/1725 (0.1%)	0.57	0/2358
2	F	0.44	3/1725 (0.2%)	0.57	0/2358
2	H	0.44	2/1725 (0.1%)	0.57	0/2358
3	I	0.48	1/3776 (0.0%)	0.75	9/5142 (0.2%)
3	J	0.56	0/3711	0.72	6/5049 (0.1%)
3	K	0.64	2/3788 (0.1%)	0.76	13/5158 (0.3%)
3	L	0.60	0/3776	0.72	7/5142 (0.1%)
3	M	0.63	2/3767 (0.1%)	0.78	11/5131 (0.2%)
3	N	0.54	0/3776	0.67	8/5142 (0.2%)
All	All	0.53	26/36326 (0.1%)	0.67	62/49452 (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
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
3	I	0	9
3	J	0	6
3	K	0	2
3	L	0	7
3	M	0	8
3	N	0	4
All	All	0	44

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	46	GLY	C-N	-5.79	1.21	1.33
1	G	97	HIS	CG-ND1	-5.50	1.32	1.38
1	C	97	HIS	CG-ND1	-5.49	1.32	1.38
1	A	97	HIS	CG-ND1	-5.47	1.32	1.38
1	E	97	HIS	CG-ND1	-5.42	1.32	1.38

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	405	GLY	N-CA-C	-15.88	86.61	110.90
3	J	429	GLN	N-CA-C	13.14	126.21	108.07
3	M	408	PRO	N-CA-C	12.04	125.39	110.70
3	K	406	LEU	N-CA-C	-8.84	96.76	109.31
3	M	408	PRO	CA-N-CD	-8.50	100.10	112.00

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	101	TYR	Peptide
2	B	181	ALA	Peptide
2	D	101	TYR	Peptide
2	D	181	ALA	Peptide
2	F	101	TYR	Peptide

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	1673	0	1625	109	0
1	C	1673	0	1625	106	0
1	E	1673	0	1625	101	0
1	G	1673	0	1625	109	0
2	B	1675	0	1620	123	0
2	D	1675	0	1620	119	0
2	F	1675	0	1620	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1675	0	1620	121	0
3	I	3675	0	3592	235	0
3	J	3614	0	3528	217	0
3	K	3686	0	3601	260	0
3	L	3675	0	3592	235	0
3	M	3666	0	3579	245	0
3	N	3675	0	3592	243	0
All	All	35383	0	34464	2194	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 31.

The worst 5 of 2194 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:M:16:VAL:HG12	3:M:17:PRO:CD	1.37	1.51
3:M:16:VAL:CG1	3:M:17:PRO:HD3	1.43	1.45
3:M:406:LEU:HA	3:M:408:PRO:HD3	1.39	1.04
2:F:100:PRO:HB2	2:F:105:THR:HG21	1.41	1.02
3:L:426:ILE:HG22	3:L:427:ALA:H	1.23	1.01

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	218/220 (99%)	192 (88%)	25 (12%)	1 (0%)	24 63
1	C	218/220 (99%)	193 (88%)	24 (11%)	1 (0%)	24 63
1	E	218/220 (99%)	192 (88%)	25 (12%)	1 (0%)	24 63
1	G	218/220 (99%)	193 (88%)	24 (11%)	1 (0%)	24 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	14	49
2	D	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	14	49
2	F	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	14	49
2	H	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	14	49
3	I	466/503 (93%)	417 (90%)	45 (10%)	4 (1%)	14	49
3	J	458/503 (91%)	424 (93%)	29 (6%)	5 (1%)	11	45
3	K	467/503 (93%)	423 (91%)	37 (8%)	7 (2%)	8	38
3	L	466/503 (93%)	424 (91%)	35 (8%)	7 (2%)	8	38
3	M	465/503 (92%)	424 (91%)	31 (7%)	10 (2%)	5	28
3	N	466/503 (93%)	434 (93%)	26 (6%)	6 (1%)	9	41
All	All	4544/4790 (95%)	4116 (91%)	377 (8%)	51 (1%)	14	45

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	408	PRO
3	K	409	PRO
3	M	17	PRO
3	N	422	THR
3	N	423	SER

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	187/187 (100%)	187 (100%)	0	100	100
1	C	187/187 (100%)	187 (100%)	0	100	100
1	E	187/187 (100%)	187 (100%)	0	100	100
1	G	187/187 (100%)	187 (100%)	0	100	100
2	B	177/177 (100%)	177 (100%)	0	100	100
2	D	177/177 (100%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	177/177 (100%)	177 (100%)	0	100	100
2	H	177/177 (100%)	177 (100%)	0	100	100
3	I	407/438 (93%)	405 (100%)	2 (0%)	81	82
3	J	399/438 (91%)	399 (100%)	0	100	100
3	K	408/438 (93%)	408 (100%)	0	100	100
3	L	407/438 (93%)	407 (100%)	0	100	100
3	M	406/438 (93%)	403 (99%)	3 (1%)	76	79
3	N	407/438 (93%)	407 (100%)	0	100	100
All	All	3890/4084 (95%)	3885 (100%)	5 (0%)	87	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	381	ILE
3	I	406	LEU
3	M	16	VAL
3	M	408	PRO
3	M	410	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	143	ASN
3	N	155	GLN
2	F	205	ASN
1	E	204	HIS
3	N	377	GLN

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 [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.

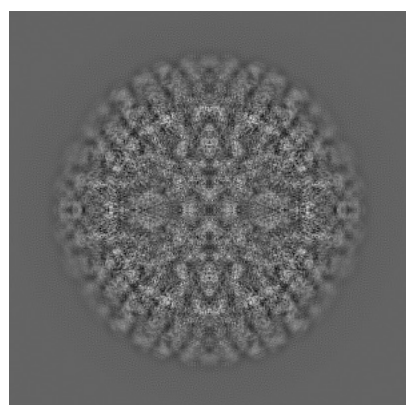
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8243. These allow visual inspection of the internal detail of the map and identification of artifacts.

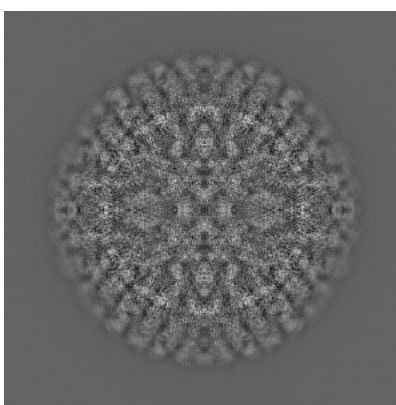
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

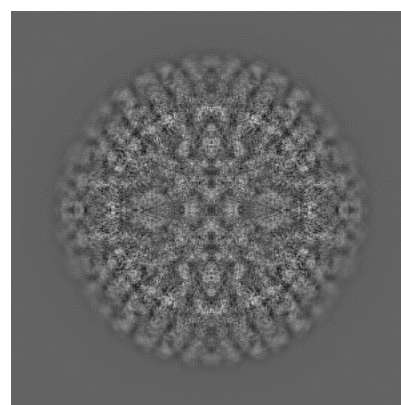
6.1.1 Primary map



X



Y

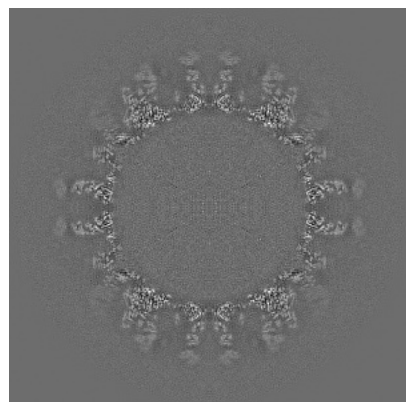


Z

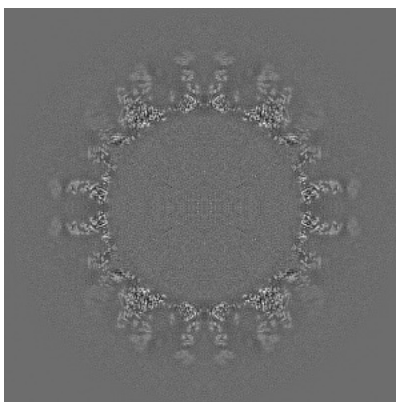
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

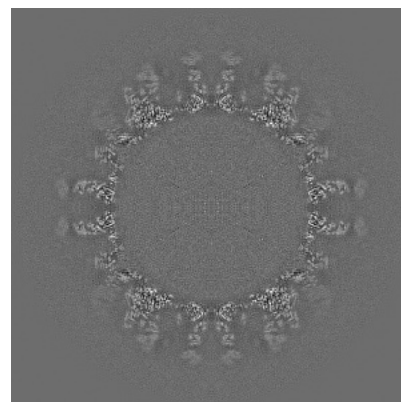
6.2.1 Primary map



X Index: 260



Y Index: 260

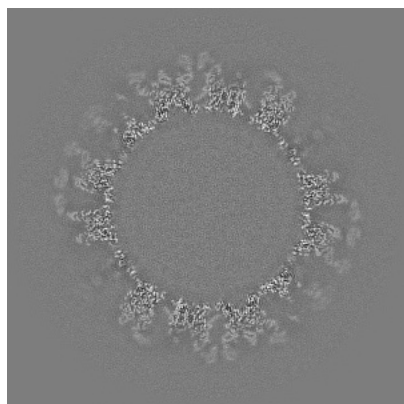


Z Index: 260

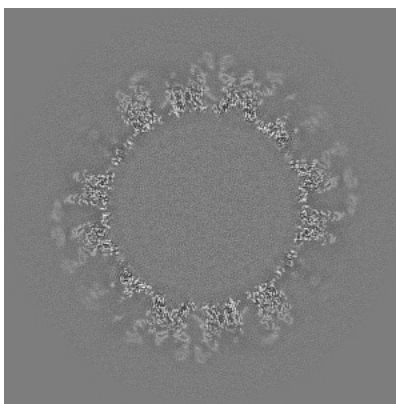
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

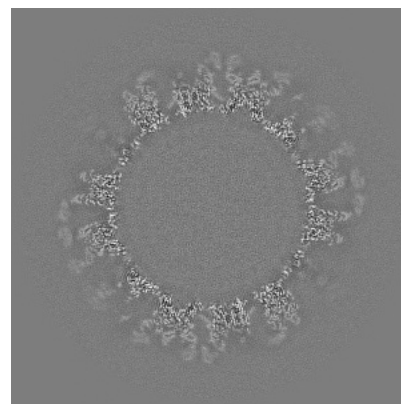
6.3.1 Primary map



X Index: 228



Y Index: 292

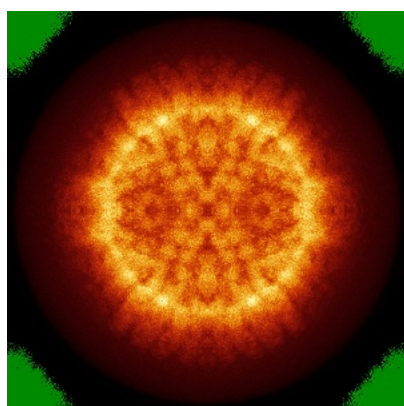


Z Index: 292

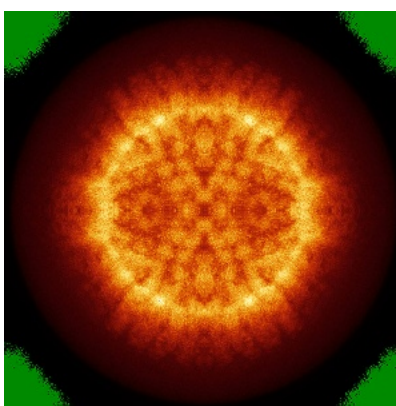
The images above show the largest variance slices of the map in three orthogonal directions.

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

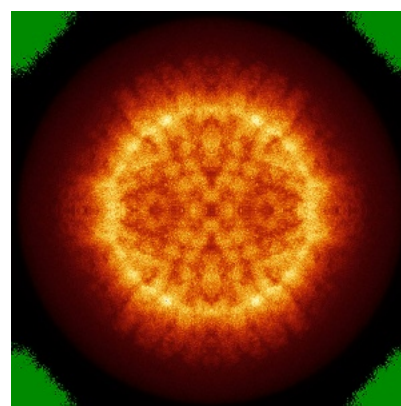
6.4.1 Primary map



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

This section was not generated.

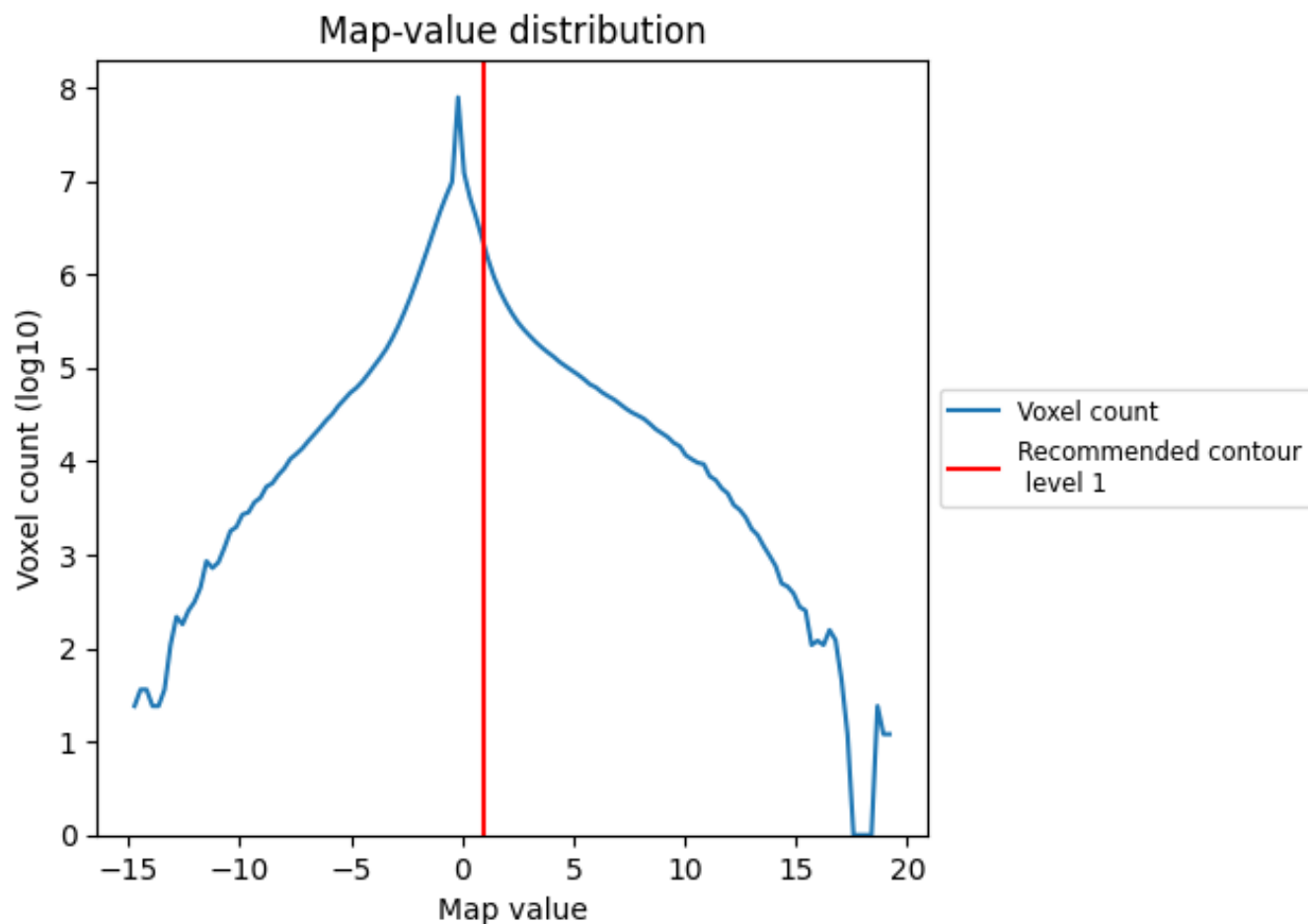
6.6 Mask visualisation

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

7 Map analysis [i](#)

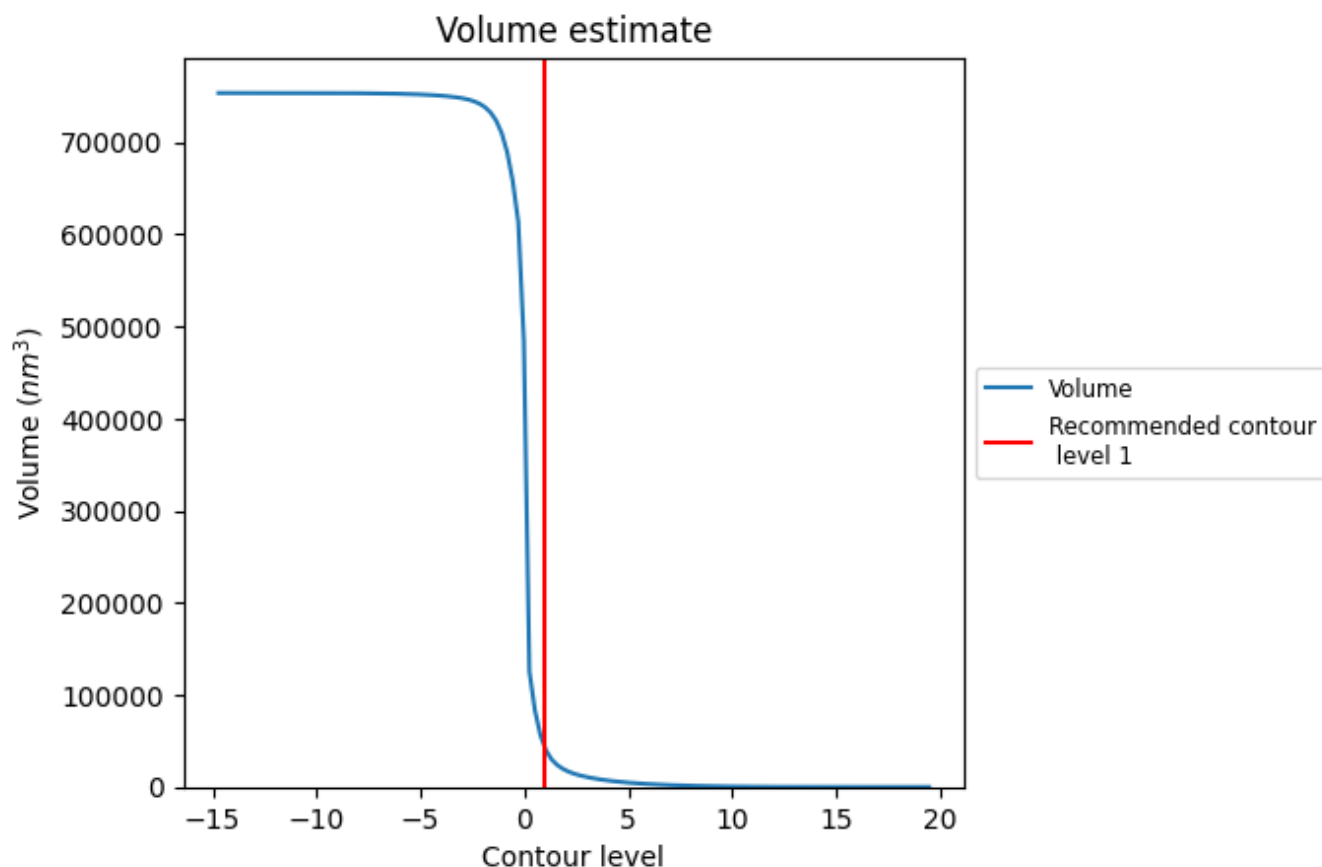
This section contains the results of statistical analysis of the map.

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.

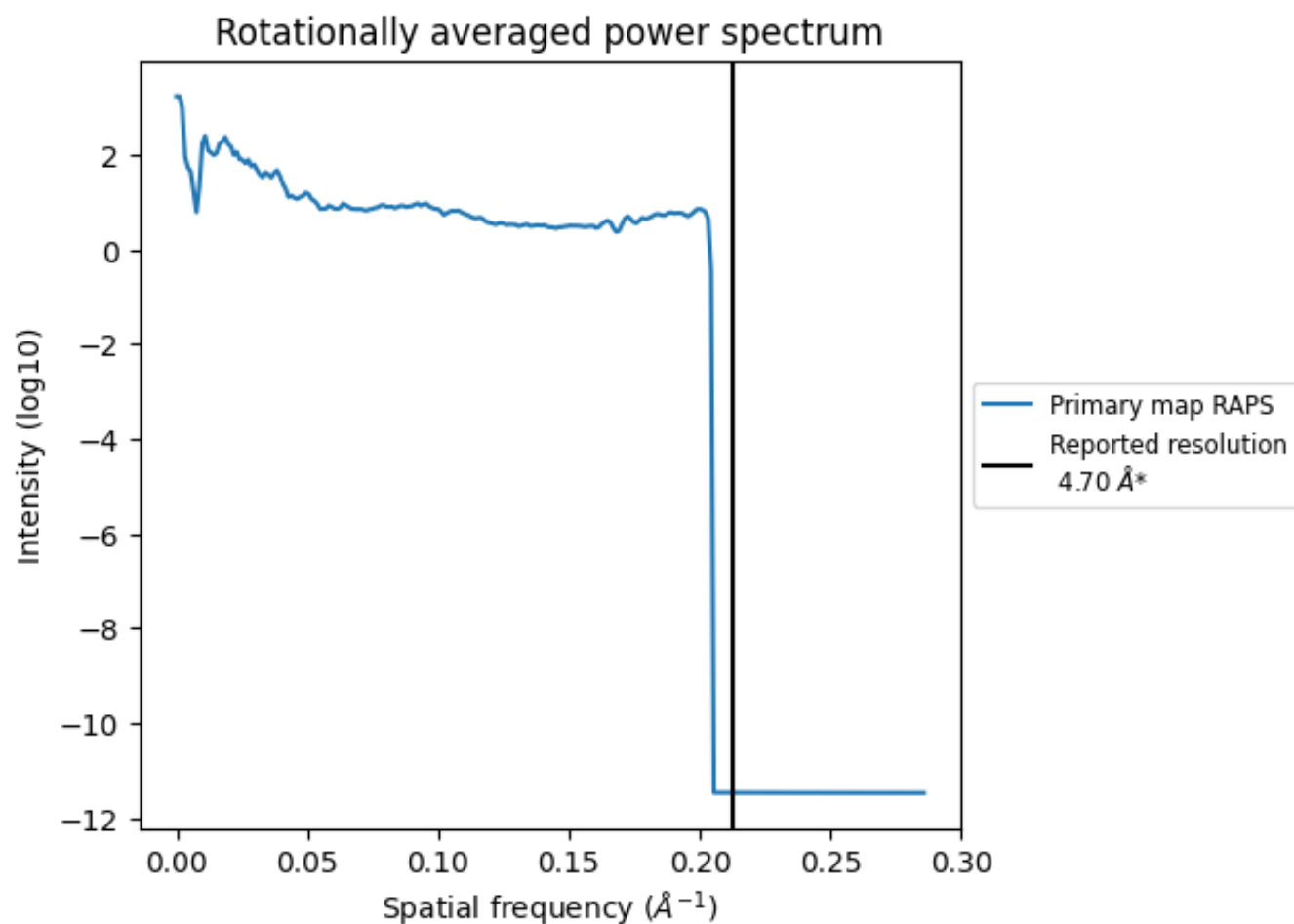
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42030 nm^3 ; this corresponds to an approximate mass of 37966 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 0.213 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

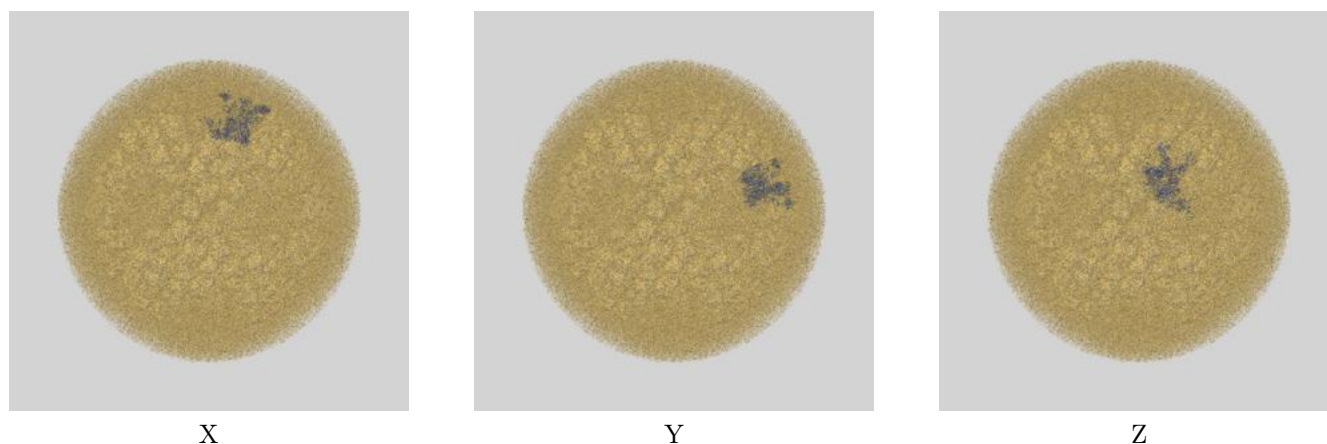
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

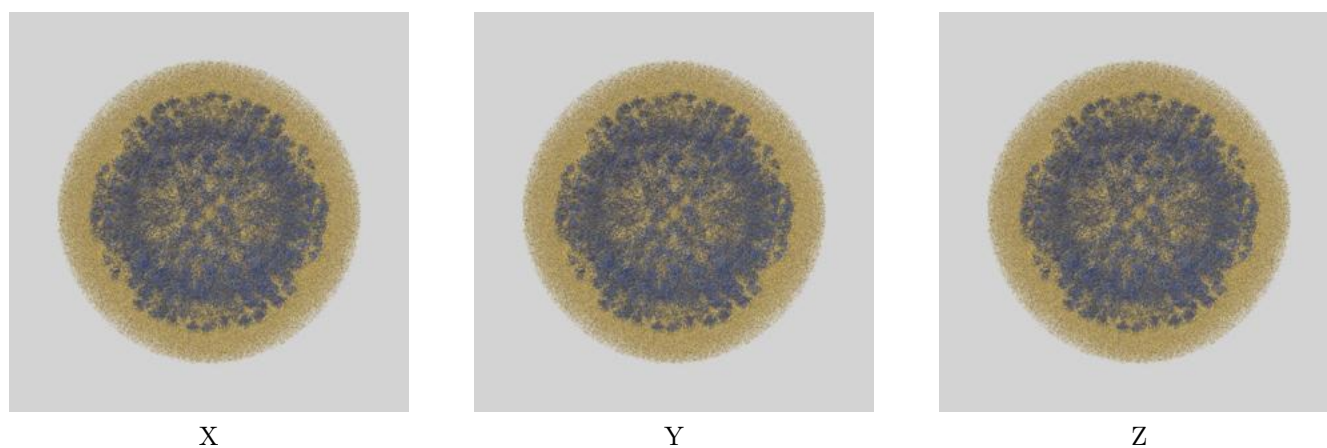
This section contains information regarding the fit between EMDB map EMD-8243 and PDB model 6BT3. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

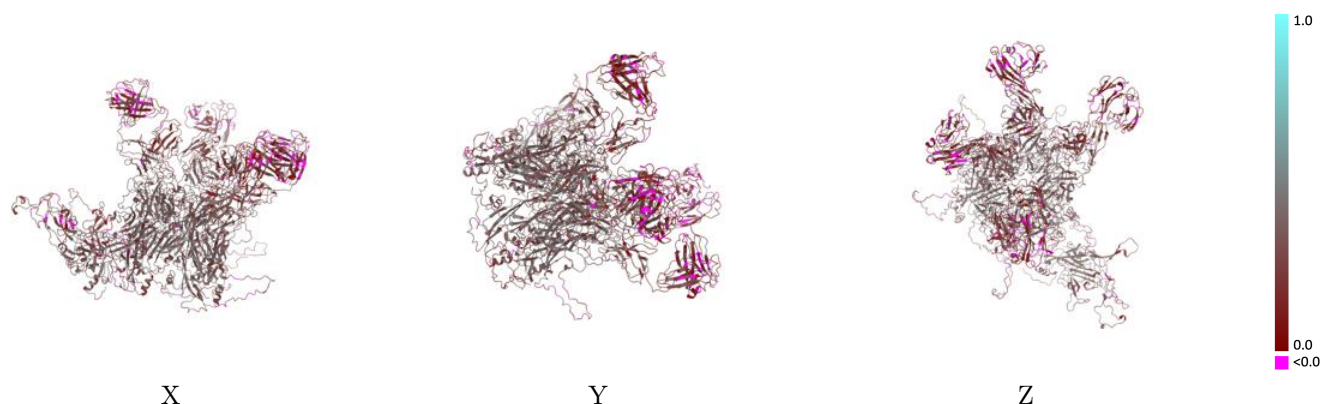


9.1.2 Map-model assembly overlay [i](#)



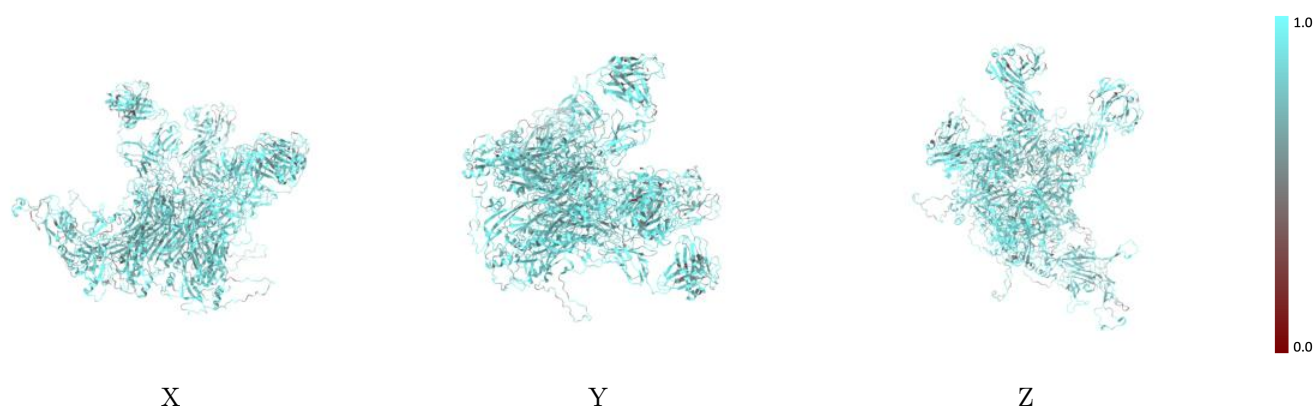
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



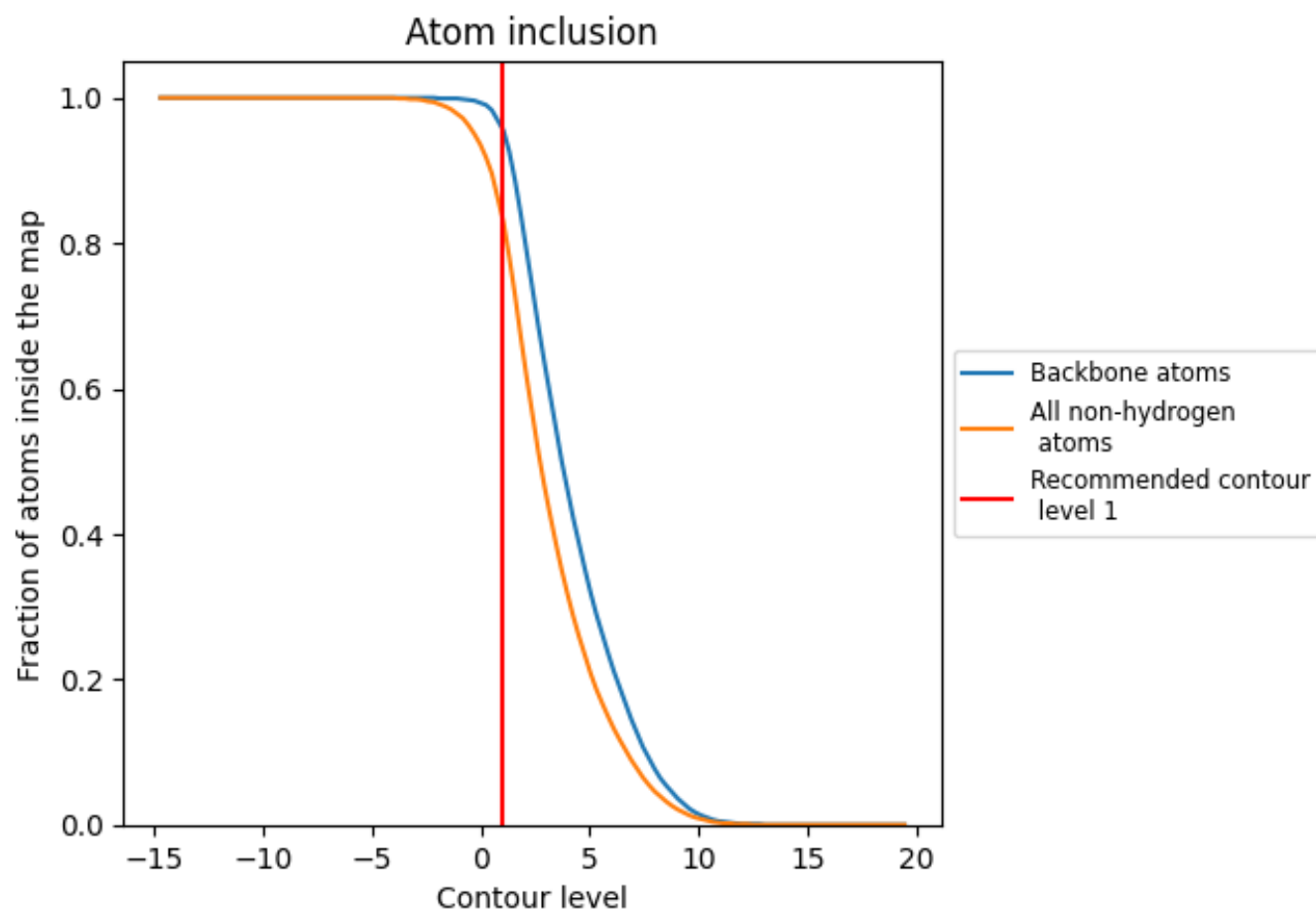
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 84% 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	 0.8350	 0.2940
A	 0.8400	 0.2130
B	 0.8500	 0.2370
C	 0.8480	 0.2150
D	 0.8470	 0.2290
E	 0.8470	 0.2240
F	 0.8350	 0.2380
G	 0.8300	 0.2140
H	 0.8420	 0.2220
I	 0.8050	 0.3070
J	 0.8360	 0.3400
K	 0.8420	 0.3440
L	 0.8460	 0.3500
M	 0.8390	 0.3470
N	 0.8200	 0.3310

