



Full wwPDB EM Validation Report

Nov 20, 2022 – 02:38 pm GMT


PDB ID : 2C8I
EMDB ID : EMD-1183
Title : Complex Of Echovirus Type 12 With Domains 1, 2, 3 and 4 Of Its Receptor Decay Accelerating Factor (Cd55) By Cryo Electron Microscopy At 16 Å
Authors : Pettigrew, D.M.; Williams, D.T.; Kerrigan, D.; Evans, D.J.; Lea, S.M.; Bhella, D.
Deposited on : 2005-12-05
Resolution : 14.00 Å (reported)
Based on initial model : 1H8T

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

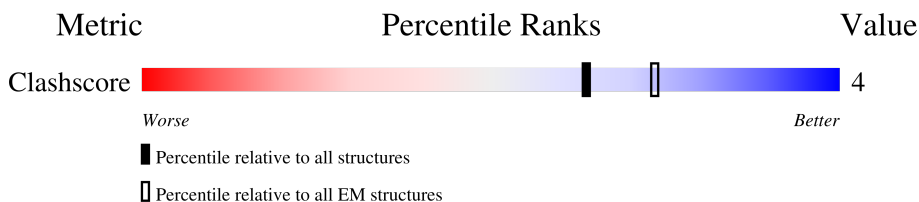
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

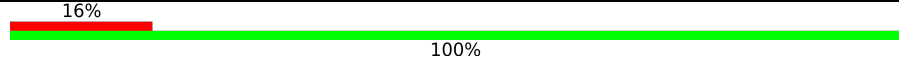
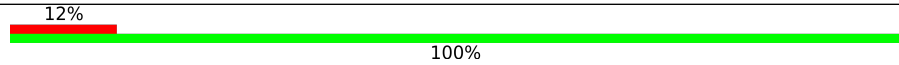
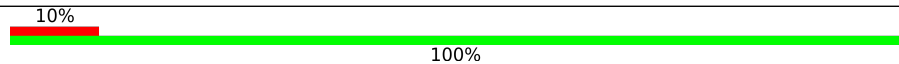
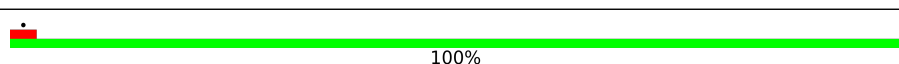

The reported resolution of this entry is 14.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297

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	289	 16% 100%
2	B	252	 12% 100%
3	C	238	 10% 100%
4	D	60	 100%
5	E	316	 80% 78% 20%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1161 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 ECHOVIRUS 11 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	289	Total	C	0	289
			289	289		

- Molecule 2 is a protein called ECHOVIRUS 11 COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	252	Total	C	0	252
			252	252		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	226	PHE	SER	conflict	UNP P29813

- Molecule 3 is a protein called ECHOVIRUS 11 COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	238	Total	C	0	238
			238	238		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	63	GLU	GLN	conflict	UNP P29813

- Molecule 4 is a protein called ECHOVIRUS 11 COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	D	60	Total	C	0	60
			60	60		

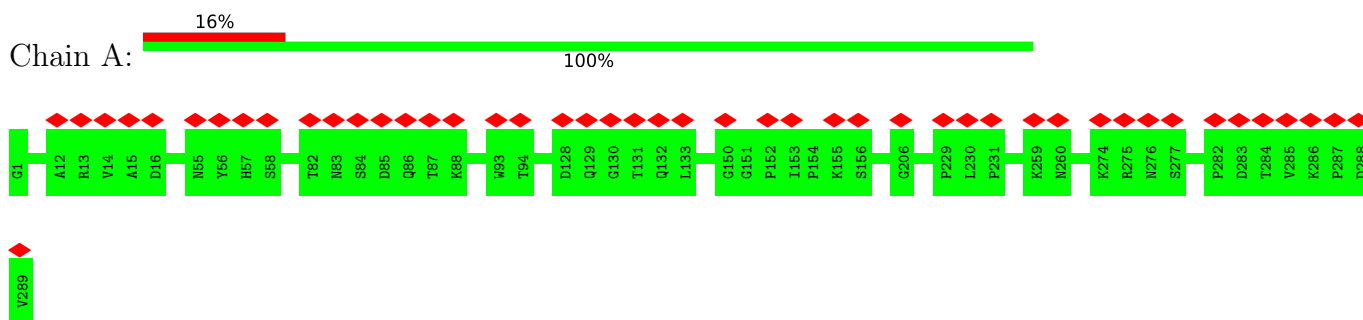
- Molecule 5 is a protein called COMPLEMENT DECAY-ACCELERATING FACTOR.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	E	252	Total 322	C 322	70	252

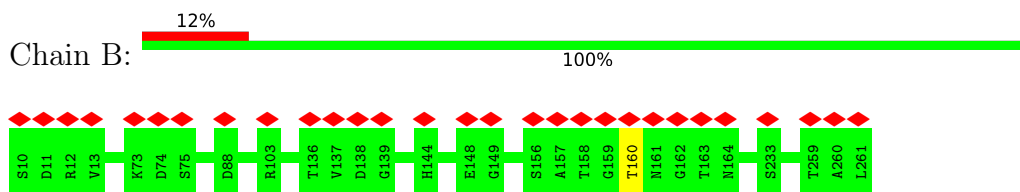
3 Residue-property plots [i](#)

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.

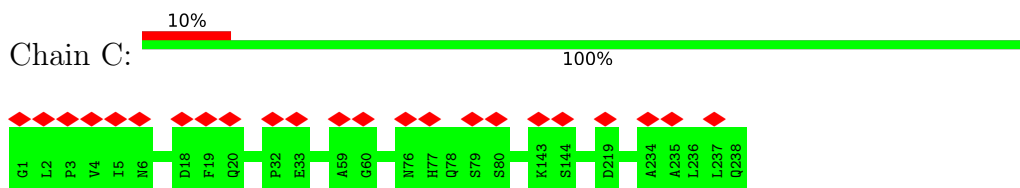
- Molecule 1: ECHOVIRUS 11 COAT PROTEIN VP1



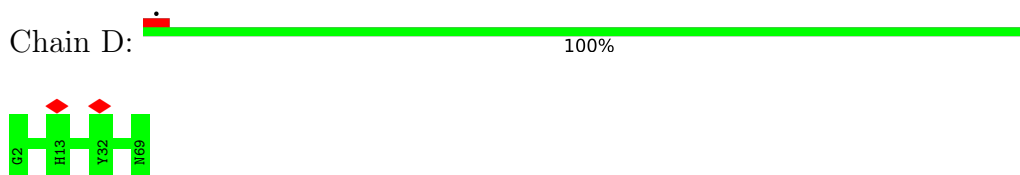
- Molecule 2: ECHOVIRUS 11 COAT PROTEIN VP2



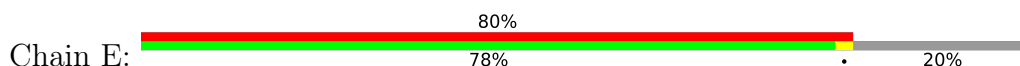
- Molecule 3: ECHOVIRUS 11 COAT PROTEIN VP3



- Molecule 4: ECHOVIRUS 11 COAT PROTEIN VP4



- Molecule 5: COMPLEMENT DECAY-ACCELERATING FACTOR



GLN	ASP	ASN	CYS	GLY	LEU	PRO	PRO	ASP	VAL	ASN	ASN	ALA	GLN	PRO	ALA	LEU	GLY	ARG	THR	SER	PHE	PRO	GLU	ASP	THR	VAL	ILE	THR	TYR	LYS	CYS	GLY	GLY	GLY	GLY	VAL	VAL	LEU	LYS	GLY	SER	GLN	TRP	SER	ASP	ILE	GLY	PHE												
CYS	ASN	ARG	SER	Q2	D3	C4	G5	L6	P7	P8	D9	V10	P11	M12	A13	Q14	P15	A16	L17	E18	G19	R20	T21	S22	F23	P24	E25	D26	T27	V28	I29	T30	Y31	K32	C33	E34	E35	S36	F37	V38	K39	I40	P41	G42	E43	K44	D45	S46	V47	I48	C49	L50	K51	G52	S53	Q54	W55	S56	D57	
I58	E59	E60	F61	C62	N63	R64	S65	C66	E67	V68	P69	T70	R71	L72	N73	S74	A75	S76	L77	K78	Q79	P80	Y81	I82	T83	Q84	N85	Y86	F87	P88	V89	G90	T91	V92	V93	E94	Y95	E96	C97	R98	P99	G100	Y101	R102	E103	R103	E104	P105	S106	L107	S108	P109	K110	L111	T112	C113	L114	Q115	N116	L117
K118	W119	S120	T121	V123	E124	F125	C126	K127	K128	K129	S130	C131	P132	N133	P134	G135	E136	I137	R138	N139	G140	Q141	I142	D143	V144	P145	G146	G147	I148	L149	F150	G151	A152	T153	I154	S155	F156	S157	C158	N159	T160	G161	Y162	K163	L164	F165	G166	S167	T168	S169	S170	F171	C172	L173	I174	S175	G176	S177		
S178	V179	Q180	W181	S182	D183	P184	L185	P186	E187	C188	R189	E190	I191	Y192	C193	P194	A195	P196	P197	Q198	I199	D200	N201	G202	I203	I204	Q205	G206	E207	R208	D209	H210	Y211	G212	Y213	R214	Q215	S216	V217	T218	Y219	A220	C221	N222	K223	G224	F225	T226	M227	I228	G229	E230	H231	S232	I233	Y234	C235	T236	V237	
N238	N239	D240	E241	G242	E243	W244	S245	G246	P247	P248	P249	E250	C251	R252	G253																																													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1501	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS PAIR IMAGES OF INDIVIDUAL PARTICLES	Depositor
Microscope	JEOL 1200	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	29100	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	445.578	Depositor
Minimum map value	-239.684	Depositor
Average map value	6.396	Depositor
Map value standard deviation	58.957	Depositor
Recommended contour level	148.0	Depositor
Map size (\AA)	555.9, 555.9, 555.9	wwPDB
Map dimensions	255, 255, 255	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2.18, 2.18, 2.18	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	289	0	0	0	0
2	B	252	0	0	1	0
3	C	238	0	0	0	0
4	D	60	0	0	0	0
5	E	322	0	0	5	0
All	All	1161	0	0	5	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 4.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:THR:CA	5:E:159:ASN:CA	2.47	0.92
5:E:18[A]:GLU:CA	5:E:19[A]:GLY:CA	2.84	0.56
5:E:18[B]:GLU:CA	5:E:19[B]:GLY:CA	2.84	0.55
5:E:79:GLN:CA	5:E:80:PRO:CA	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:PRO:CA	5:E:100:GLY:CA	2.88	0.52

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

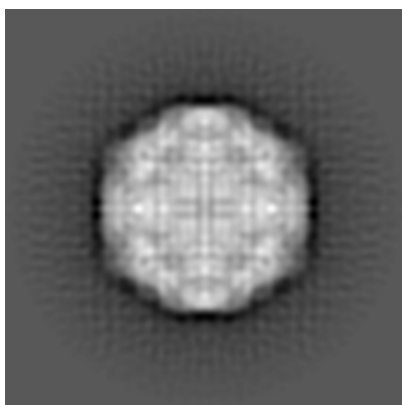
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1183. These allow visual inspection of the internal detail of the map and identification of artifacts.

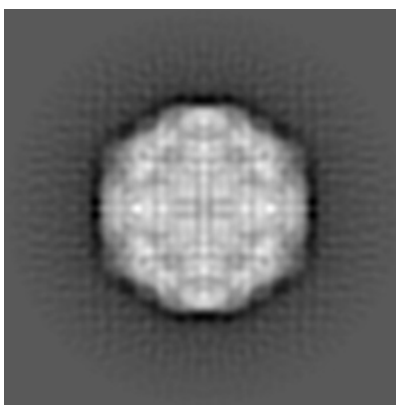
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

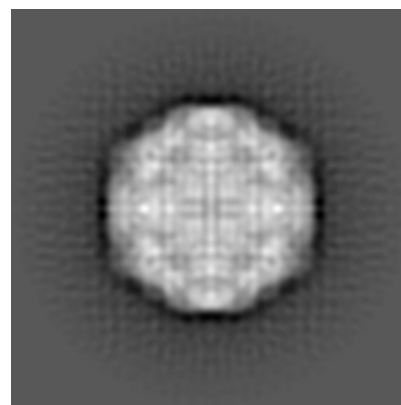
6.1.1 Primary map



X



Y

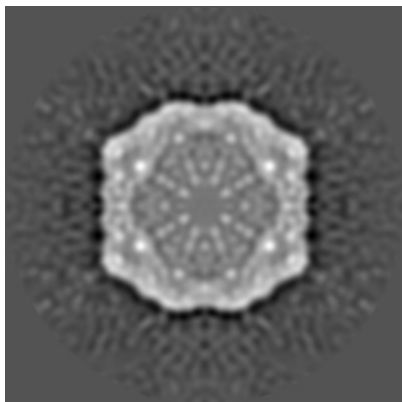


Z

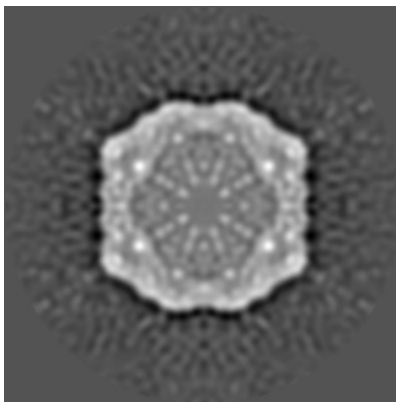
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

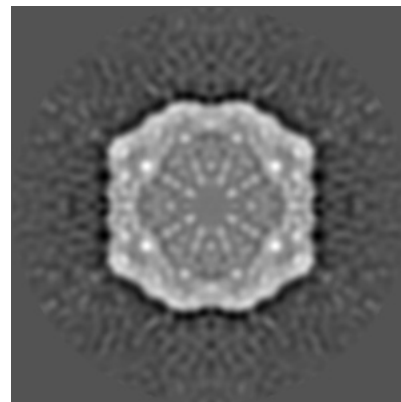
6.2.1 Primary map



X Index: 127



Y Index: 127

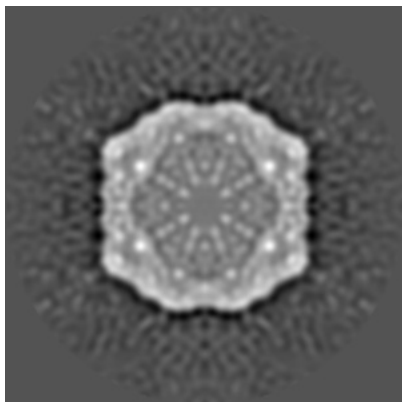


Z Index: 127

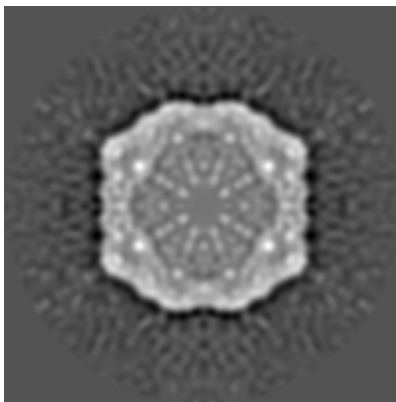
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

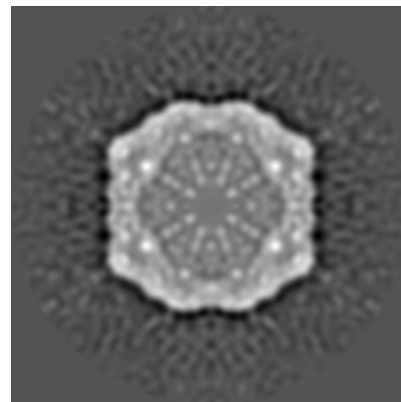
6.3.1 Primary map



X Index: 127



Y Index: 127

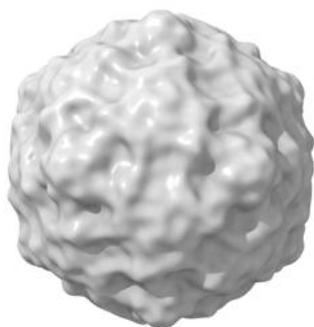


Z Index: 127

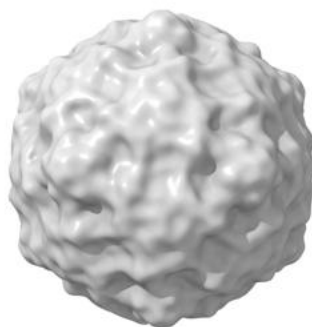
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

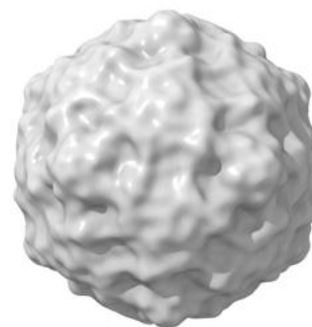
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 148.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

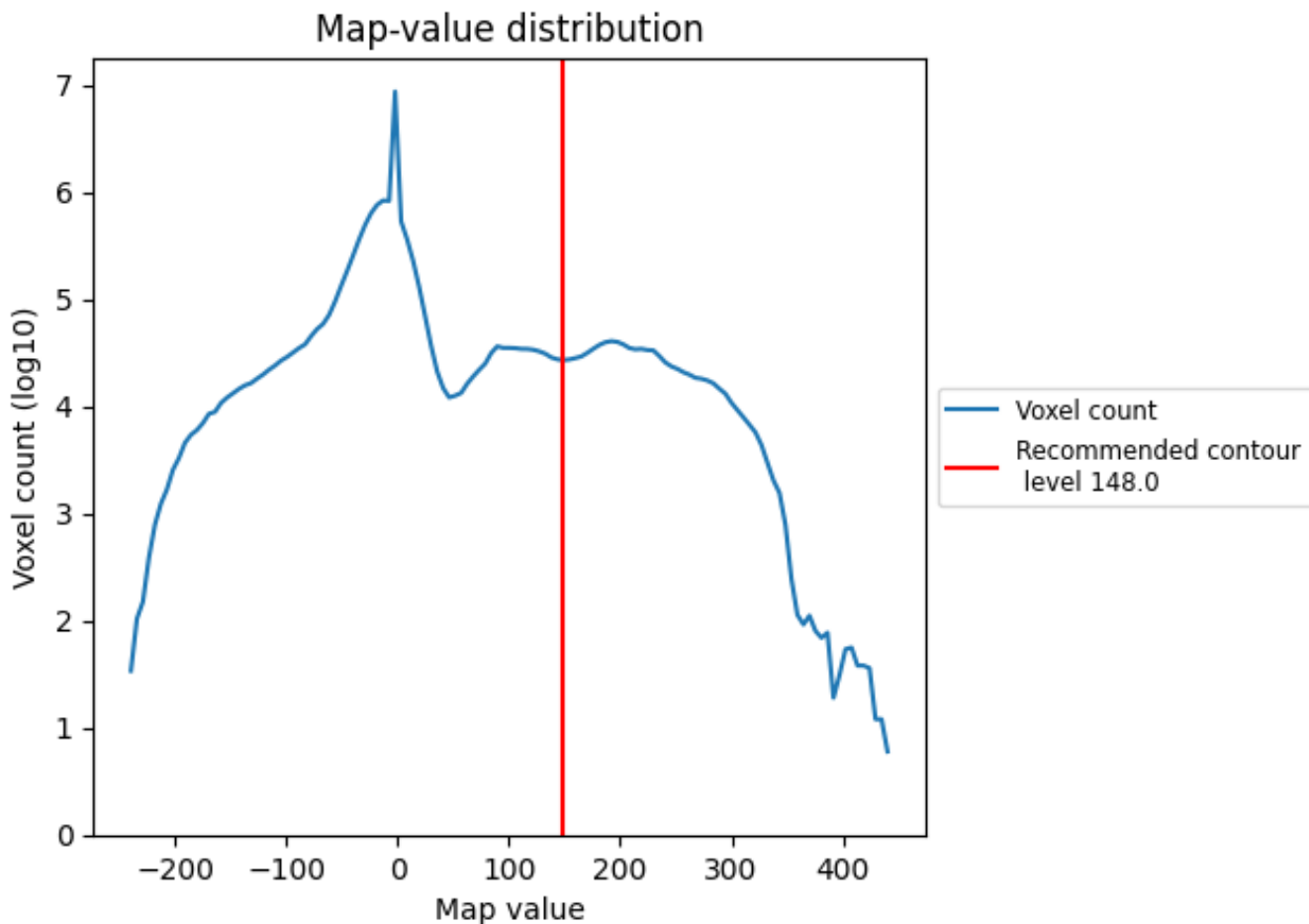
6.5 Mask visualisation

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

7 Map analysis [i](#)

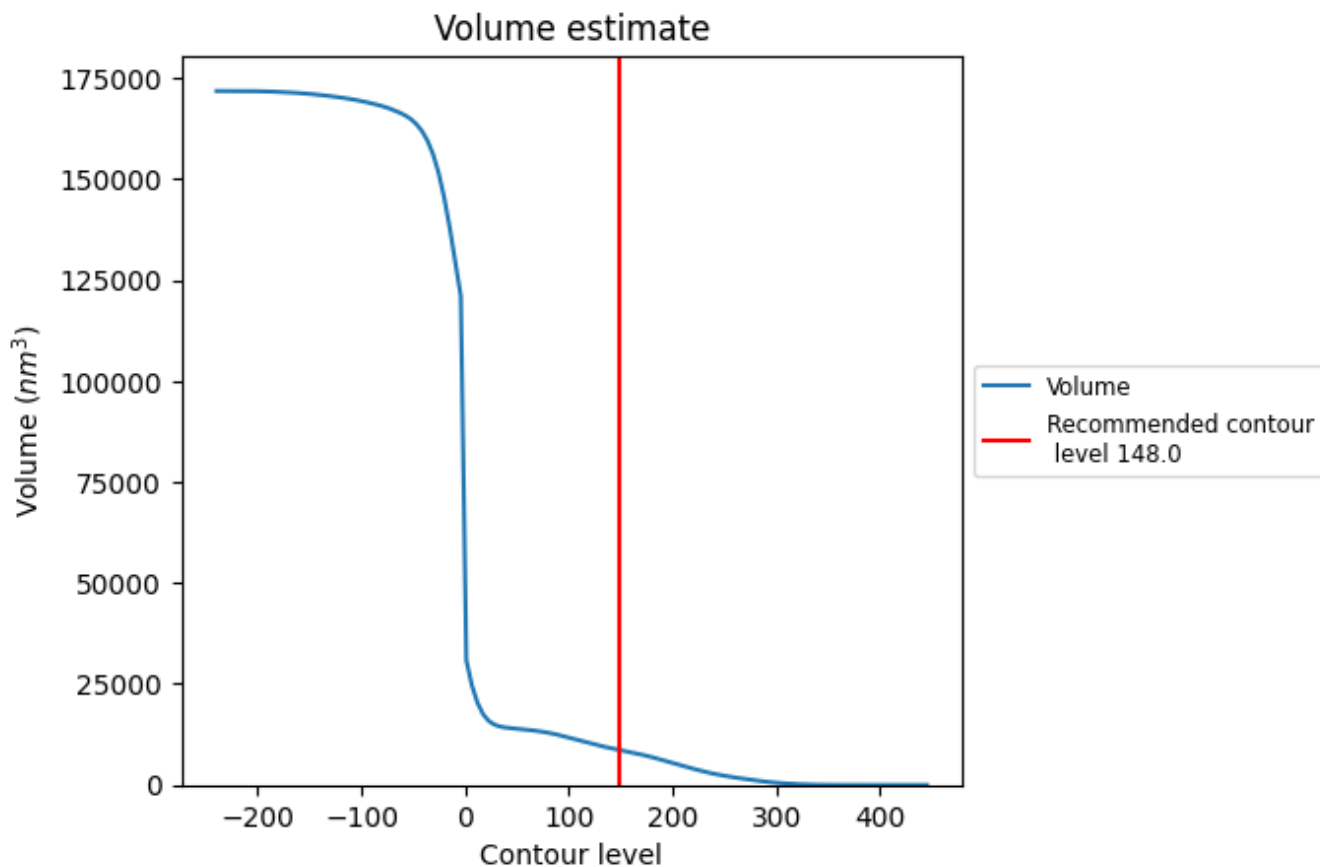
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

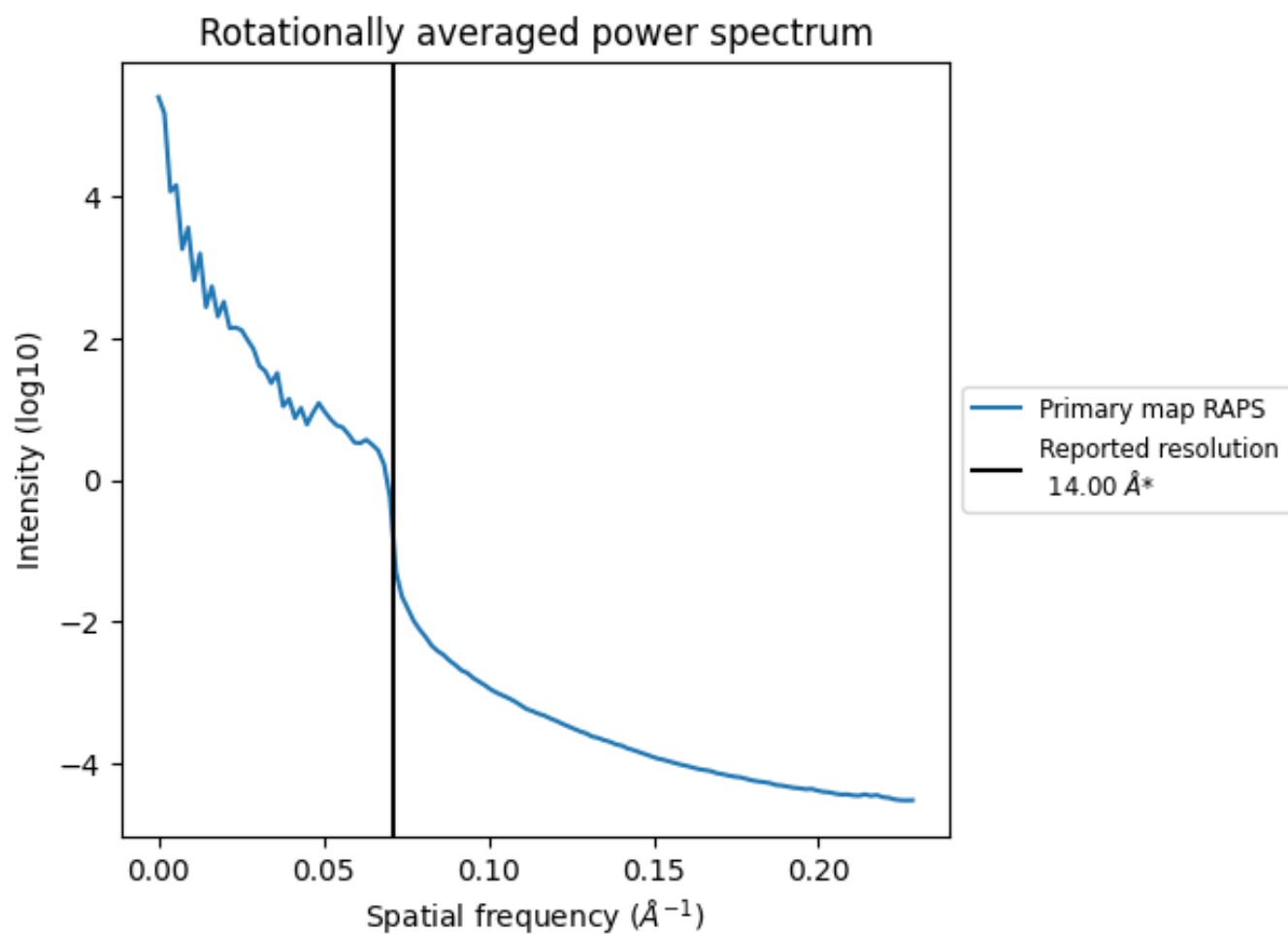
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 8698 nm³; this corresponds to an approximate mass of 7857 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 0.071\AA^{-1}

8 Fourier-Shell correlation

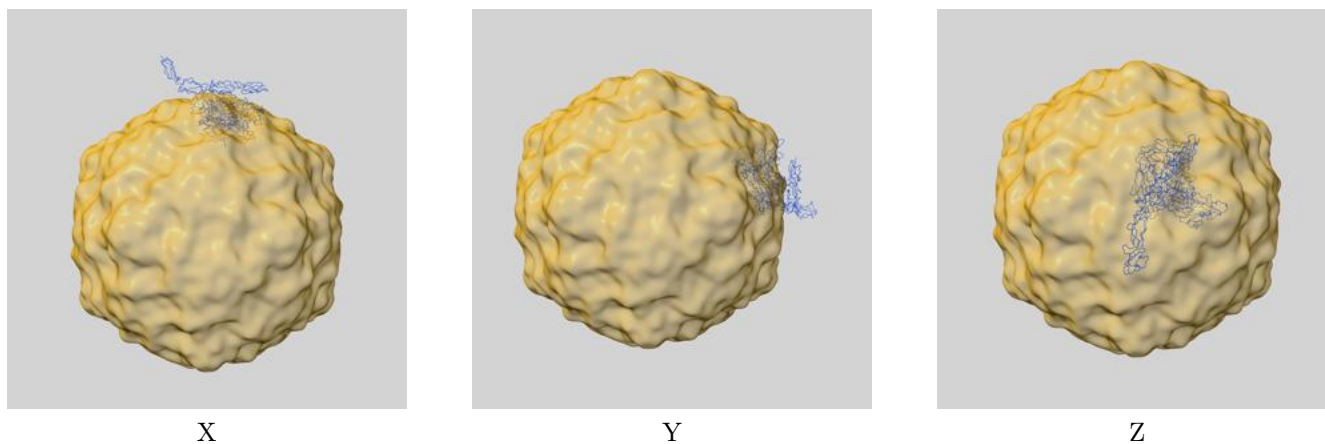
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

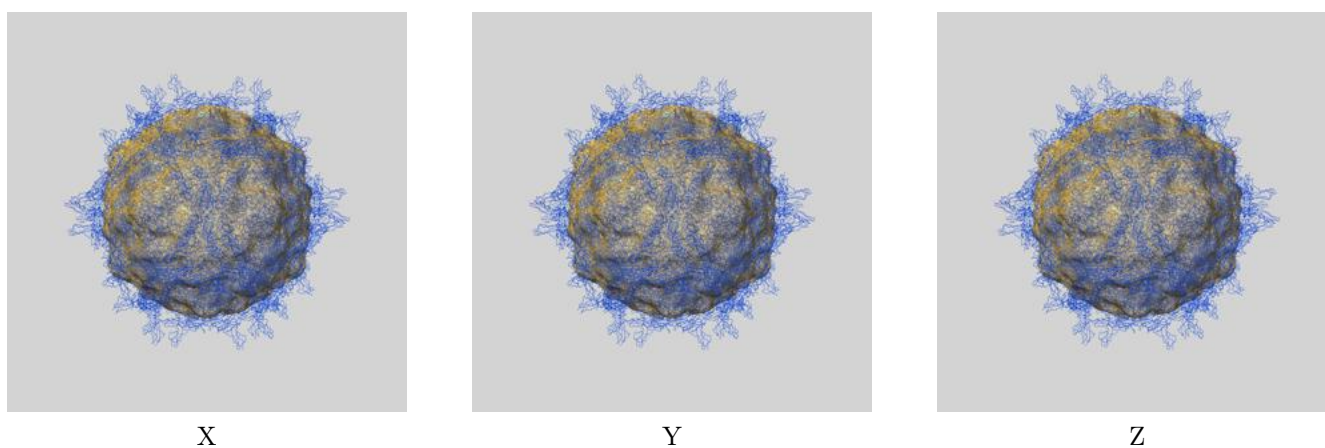
This section contains information regarding the fit between EMDB map EMD-1183 and PDB model 2C8I. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

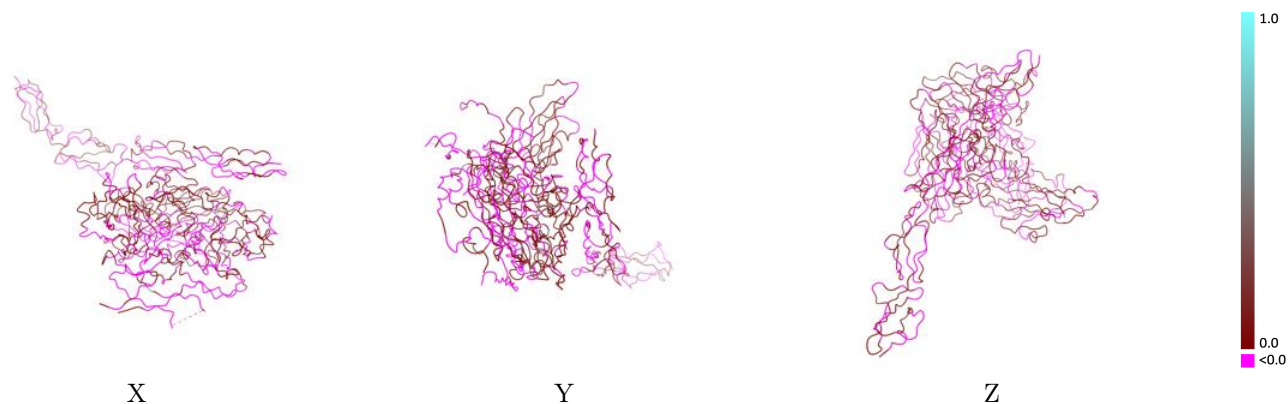


9.1.2 Map-model assembly overlay [i](#)



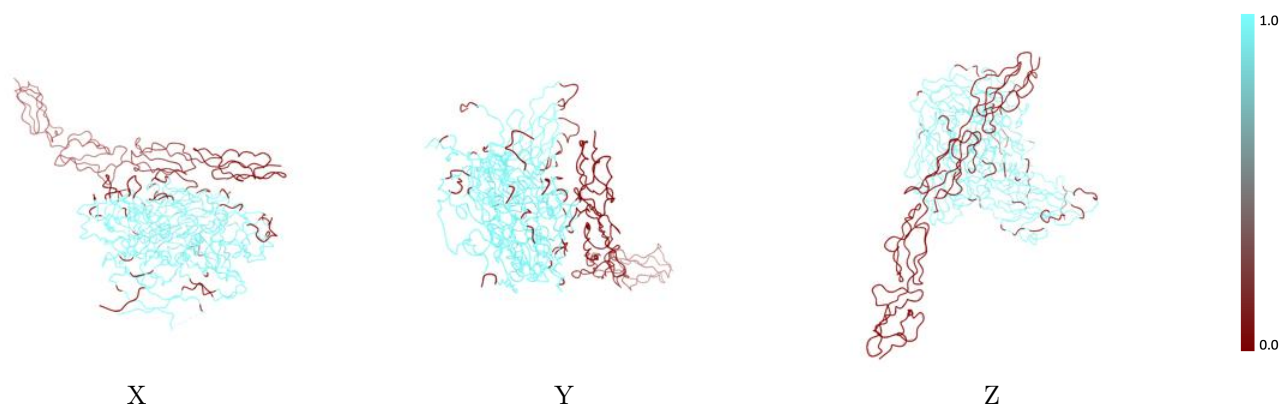
The images above show the 3D surface view of the map at the recommended contour level 148.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



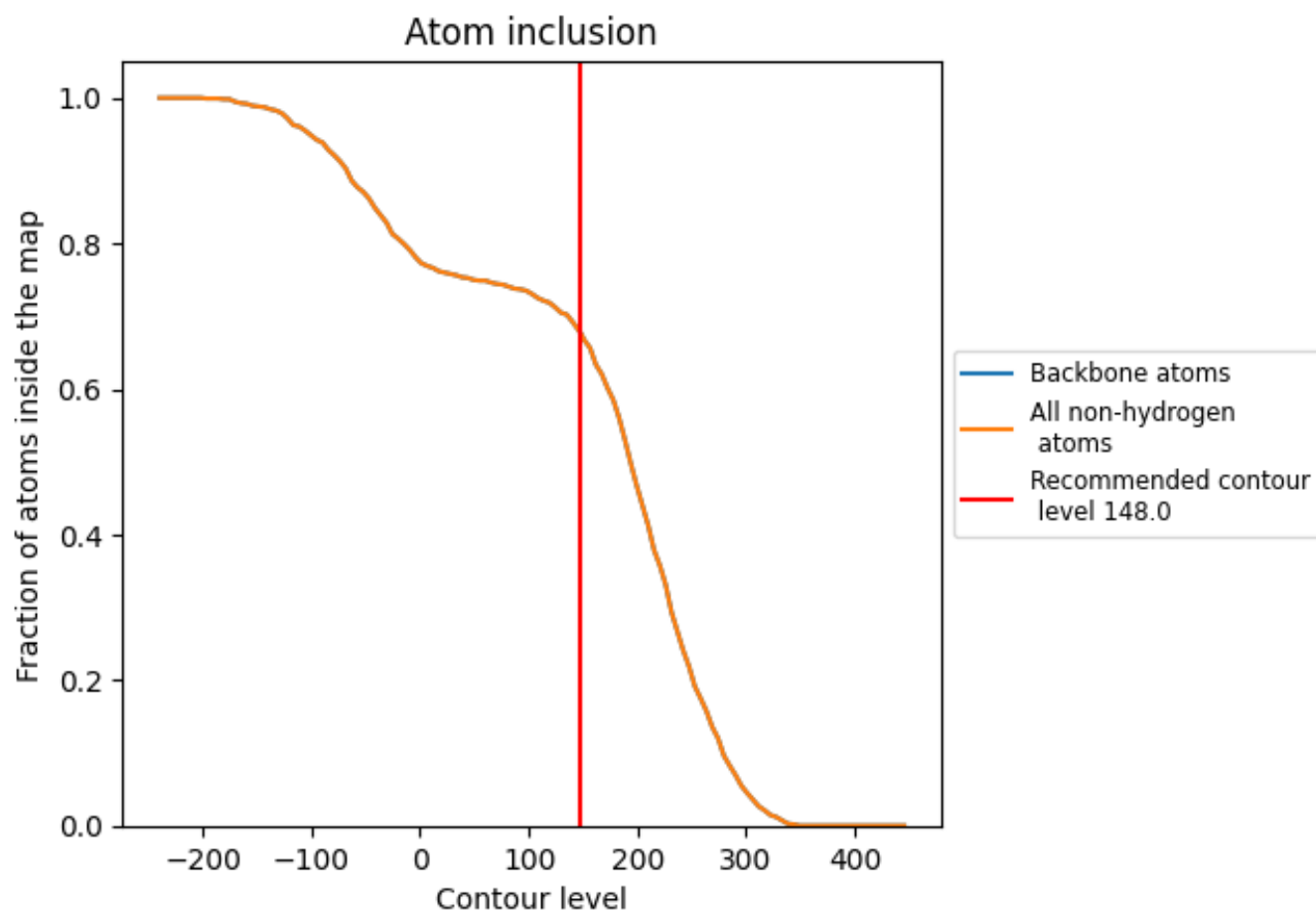
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (148.0).













9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (148.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6764	 0.0110
A	 0.8374	 0.0170
B	 0.8849	 0.0220
C	 0.9034	 0.0280
D	 0.9667	 -0.0400
E	 0.0000	 -0.0090

