wwPDB EM Validation Summary Report (i)

Nov 8, 2022 – 08:12 PM EST

PDB ID	:	6MW9
EMDB ID	:	EMD-9274
Title	:	CryoEM structure of chimeric Eastern Equine Encephalitis Virus with Fab of EEEV-3 antibody
Authors	:	Hasan, S.S.; Sun, C.; Kim, A.S.; Watanabe, Y.; Chen, C.L.; Klose, T.; Buda, G.; Crispin, M.; Diamond, M.S.; Klimstra, W.B.; Rossmann, M.G.
Deposited on	:	2018-10-29
Resolution	:	7.30 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 (i) 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 (i)) were used in the production of this report:

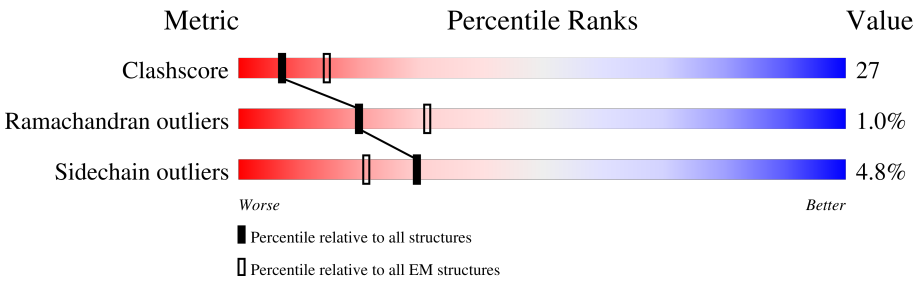
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	441	• 70% 20% • 9%
1	E	441	6% 71% 19% • 9%
1	I	441	• 70% 20% • 9%
1	M	441	7% 71% 19% • 9%
2	B	420	63% 15% 23%
2	F	420	• 60% 17% 23%
2	J	420	• 61% 16% 23%
2	N	420	5% 61% 16% 23%

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Mol	Chain	Length	Quality of chain
3	C	218	6% 58% 38%
3	G	218	60% 35%
3	K	218	5% 58% 38%
3	O	218	60% 36%
4	D	214	8% 43% 42% 13%
4	H	214	6% 41% 44% 13%
4	L	214	8% 44% 41% 12%
4	P	214	6% 45% 40% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35528 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	400	3063	1940	511	592	20	0	0
1	E	400	3063	1940	511	592	20	0	0
1	I	400	3063	1940	511	592	20	0	0
1	M	400	3063	1940	511	592	20	0	0

- Molecule 2 is a protein called E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	325	2550	1601	471	462	16	0	0
2	F	325	2550	1601	471	462	16	0	0
2	J	325	2550	1601	471	462	16	0	0
2	N	325	2550	1601	471	462	16	0	0

- Molecule 3 is a protein called EEEV-3 antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	218	1671	1066	272	326	7	0	0
3	G	218	1671	1066	272	326	7	0	0
3	K	218	1671	1066	272	326	7	0	0
3	O	218	1671	1066	272	326	7	0	0

- Molecule 4 is a protein called EEEV-3 antibody light chain.

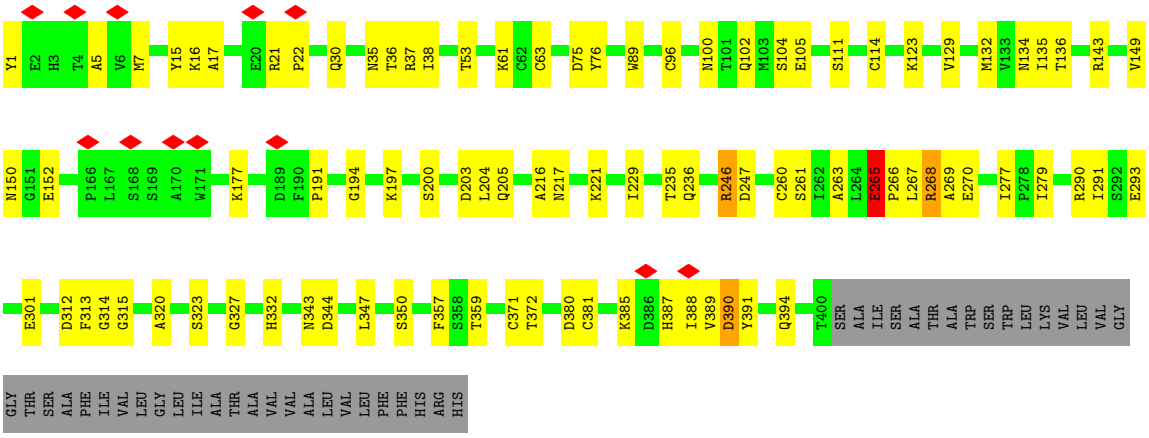
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	211	1598	999	270	322	7	0	0
4	H	211	1598	999	270	322	7	0	0
4	L	211	1598	999	270	322	7	0	0
4	P	211	1598	999	270	322	7	0	0

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.

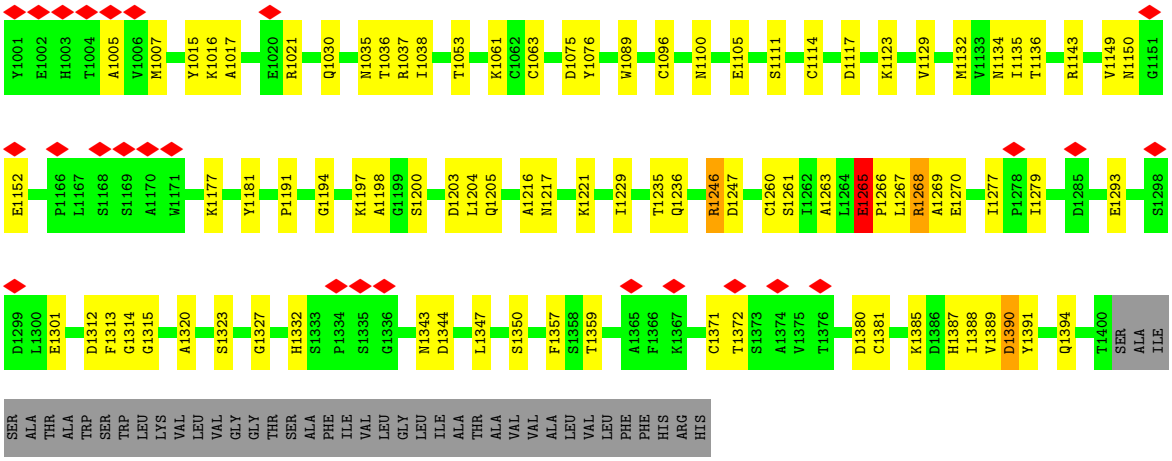
- Molecule 1: E1

Chain A:



- Molecule 1: E1

Chain E:



- Molecule 1: E1

Chain I: 70% 20% • 9%

Y2001 A2005 V2006 M2007 G2012 Y2015 K2016 A2017 R2021 Q2030 N2035 T2036 R2037 I2038 T2053 S2057 K2061 C2062 C2063 Q2067 C2068 T2069 S2070 D2075 Y2076 Q2079 W2089 C2096 N2100 E2105 S2111 C2114 D2117 V2129 M2132 V2133 N2134 I2135 T2136

R2143 V2149 E2152 S2168 S2169 A2170 W2171 D2175 N2176 Y2181 D2189 F2190 P2191 G2194 K2197 A2198 G2199 S2200 D2203 L2204 Q2205 A2216 N2217 K2221 I2229 T2235 Q2236 R2246 D2247 C2260 S2261 I2262 A2263 L2264 E2265 P2266 L2267 R2268 A2269 E2270 I2279 E2293

E2301 C2302 K2303 E2306 D2312 F2313 G2314 G2315 I2316 A2320 S2323 G2327 H2332 N2343 D2344 L2347 S2350 H2356 F2357 S2358 T2359 C2371 T2372 D2380 C2381 K2382 K2385 D2386 H2387 I2388 V2389 D2390 Y2391 Q2394 T2400 SER ALA ILE SER ALA THR ALA TRP SER

TRP LEU LYS VAL LEU VAL GLY GLY THR SER ALA PHE ILE VAL LEU GLY LEU ILE ALA THR ALA VAL VAL ALA LEU VAL LEU PHE PHE HIS ARG HIS

• Molecule 1: E1

Chain M: 7% 71% 19% • 9%

Y3001 E3002 H3003 T3004 A3005 V3006 M3007 P3008 Y3015 K3016 A3017 E3020 R3021 Q3030 N3035 T3036 R3037 I3038 T3053 K3061 C3062 C3063 S3070 D3075 Y3076 W3089 C3096 N3100 T3101 Q3102 M3103 S3104 E3105 S3111 C3114 T3126 V3129 M3132 V3133 N3134 I3135 T3136 R3143

V3149 E3152 P3166 L3167 S3168 S3169 A3170 W3171 D3175 N3176 K3177 N3187 Y3188 D3189 P3190 P3191 G3194 K3197 A3198 G3199 S3200 D3203 L3204 Q3205 A3216 N3217 K3221 I3229 T3235 Q3236 R3246 D3247 K3248 G3249 C3260 S3261 I3262 A3263 L3264 E3265 P3266 L3267 R3268 A3269 E3270

V3274 G3275 S3276 I3277 P3278 I3279 E3293 D3299 L3300 E3301 D3312 F3313 G3314 G3315 A3320 S3323 G3327 H3332 S3335 G3336 N3343 D3344 L3347 S3350 F3357 S3358 T3359 A3365 C3371 T3372 T3376 D3380 C3381 K3385 D3386 H3387 I3388 V3389 D3390 Y3391 Q3394

T3400 SER ALA ILE SER ALA THR ALA TRP SER TRP LEU LYS VAL LEU VAL GLY GLY THR SER ALA PHE ILE VAL LEU GLY LEU ILE ALA THR ALA VAL VAL ALA LEU VAL LEU PHE PHE HIS ARG HIS

• Molecule 2: E2

Chain B: 63% 15% 23%

ASP LEU ASP THR HIS PHE THR GLN TYR LYS LEU ALA ARG P501 Y502 I503 A504 D505 N508 R513 C514 D515 G530 R533 S537 L542 M552 N556 I563 D566 N567 L568 H569 V570 R571 S577 H581 H582 G583 Q589 C590 T595 V596 T597 V598 G599

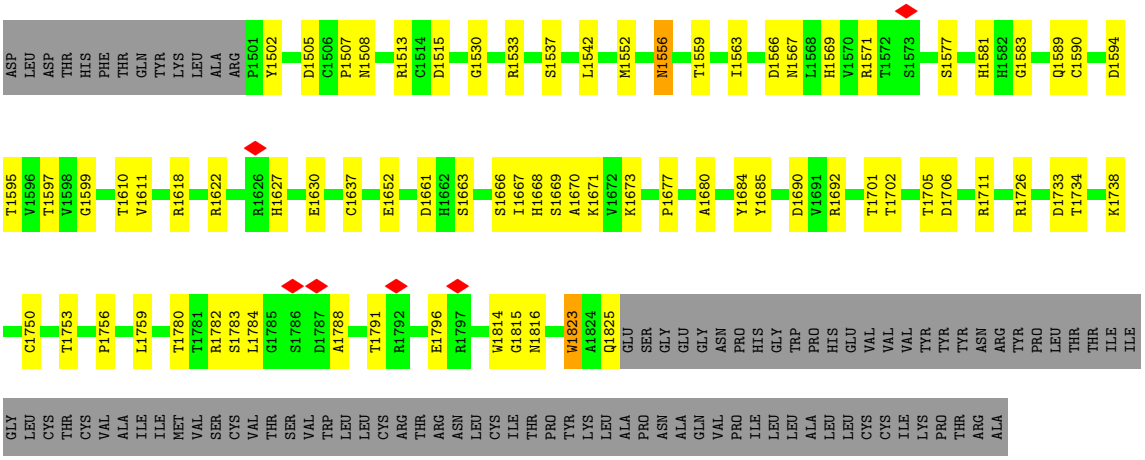
T610 V611 R618 R622 R626 E652 S666 I667 H668 S669 A670 K671 V672 K673 P677 A680 Y684 Y685 D690 V691 R692 T701 T702 T705 R711 R726 D733 T734 K738 T753 P756 R782 S783 L784 A788 E796 R797 W814

G815 N816 W823 A824 Q825 GLU SER GLY GLU GLY ASN PRO HIS GLY TRP PRO HIS GLU VAL VAL VAL TYR TYR TYR TYR ASN ARG TYR PRO LEU THR THR ILE ILE GLY LEU CYS THR CYS VAL ALA ILE ILE MET VAL SER CYS VAL THR SER VAL TRP LEU LEU CYS ARG THR ARG ASN LEU

CYS ILE THR PRO TYR LYS LEU ALA PRO ASN ALA GLN VAL PRO ILE LEU LEU ALA LEU LEU CYS CYS ILE LYS PRO THR ARG ALA

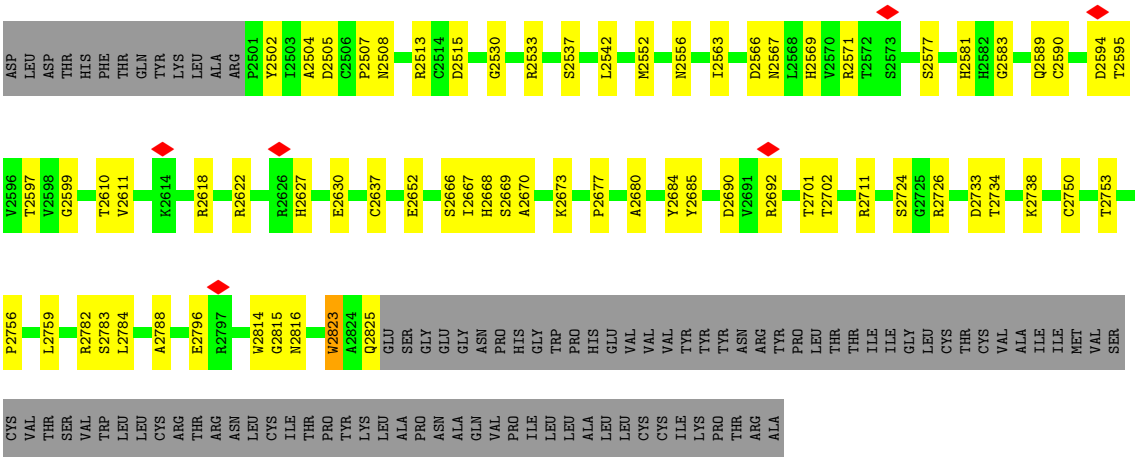
- Molecule 2: E2

Chain F:



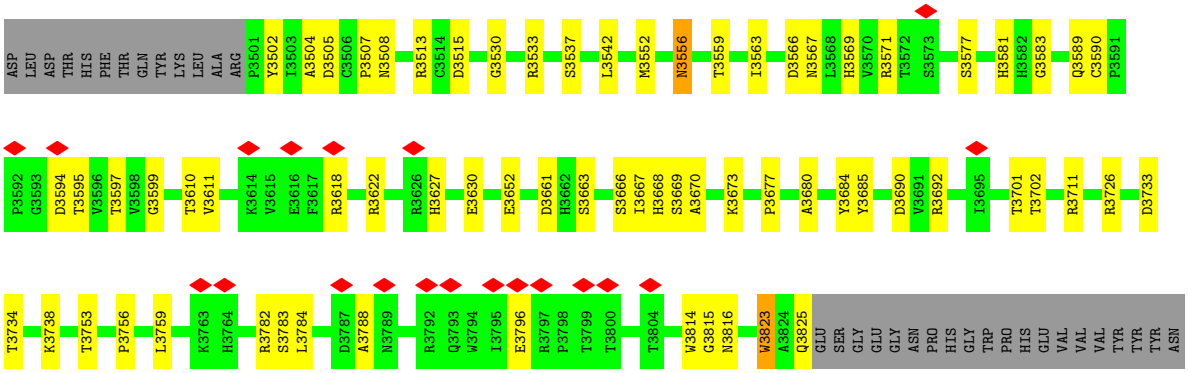
- Molecule 2: E2

Chain J:



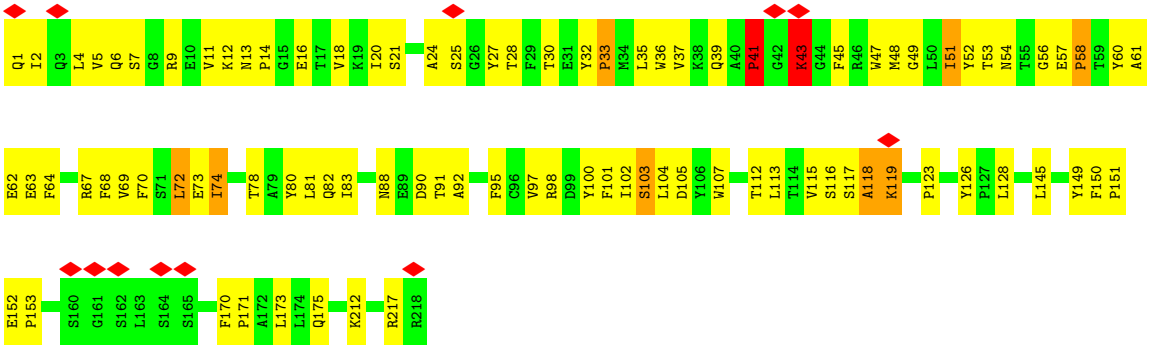
- Molecule 2: E2

Chain N:



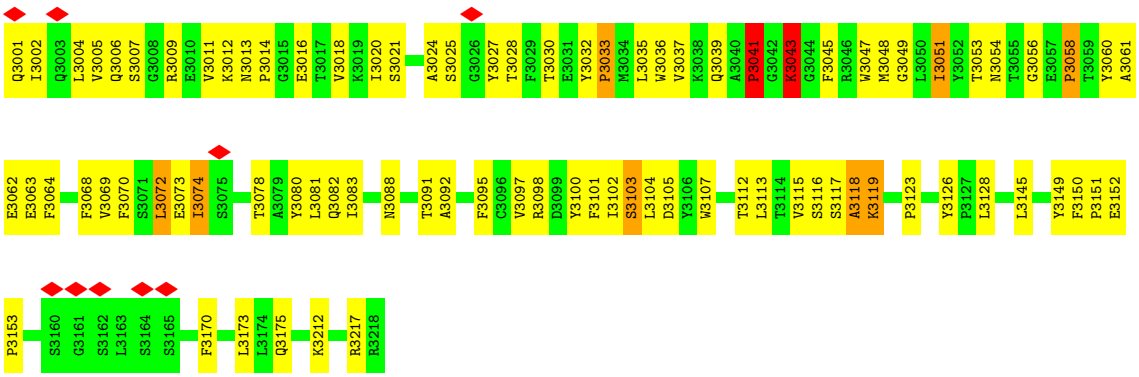
• Molecule 3: EEEV-3 antibody heavy chain

Chain C:



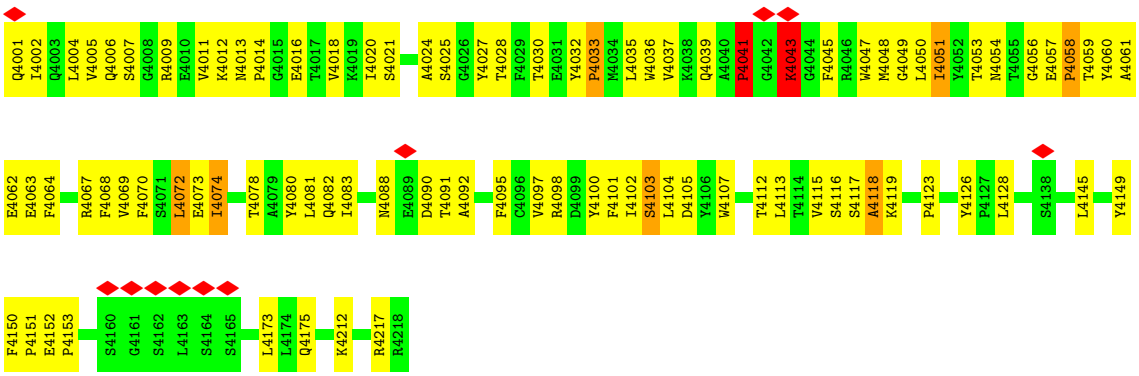
• Molecule 3: EEEV-3 antibody heavy chain

Chain G:



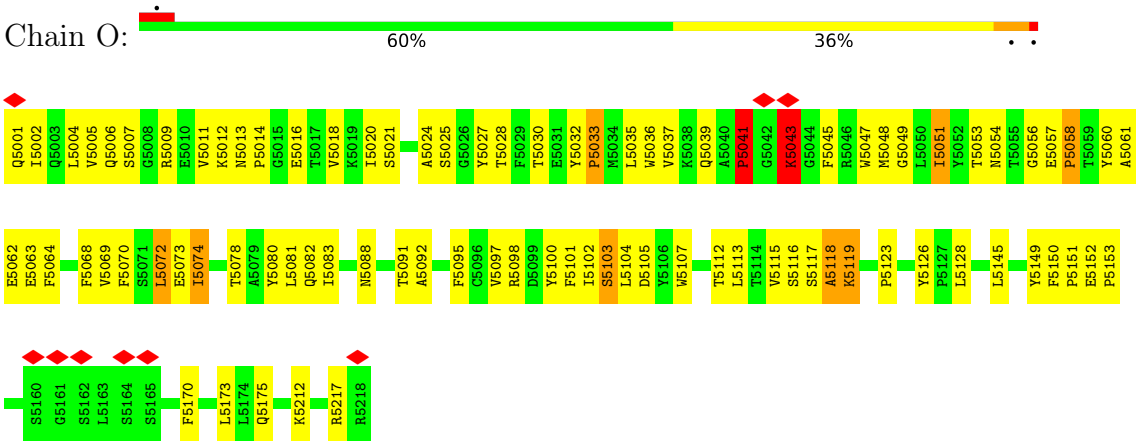
• Molecule 3: EEEV-3 antibody heavy chain

Chain K:



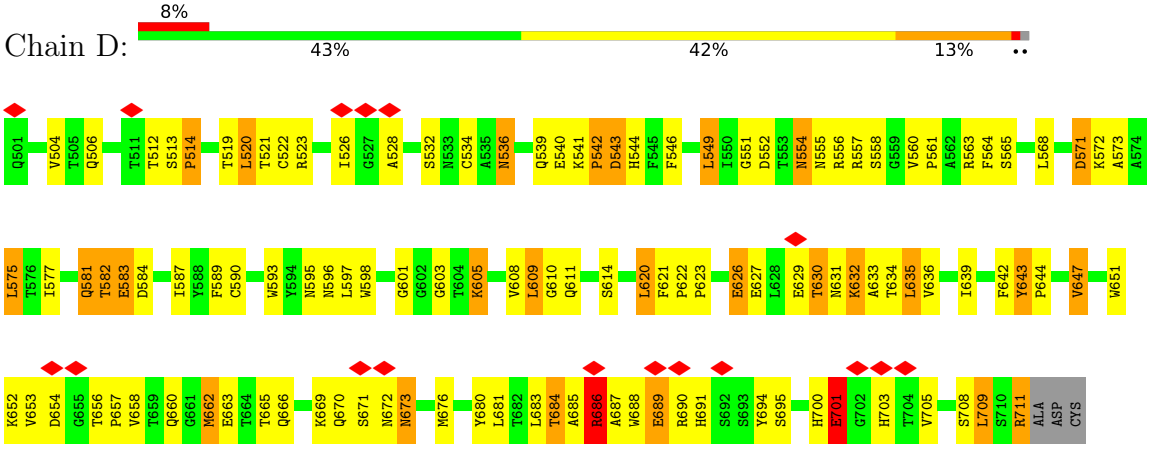
- Molecule 3: EEEV-3 antibody heavy chain

Chain O:



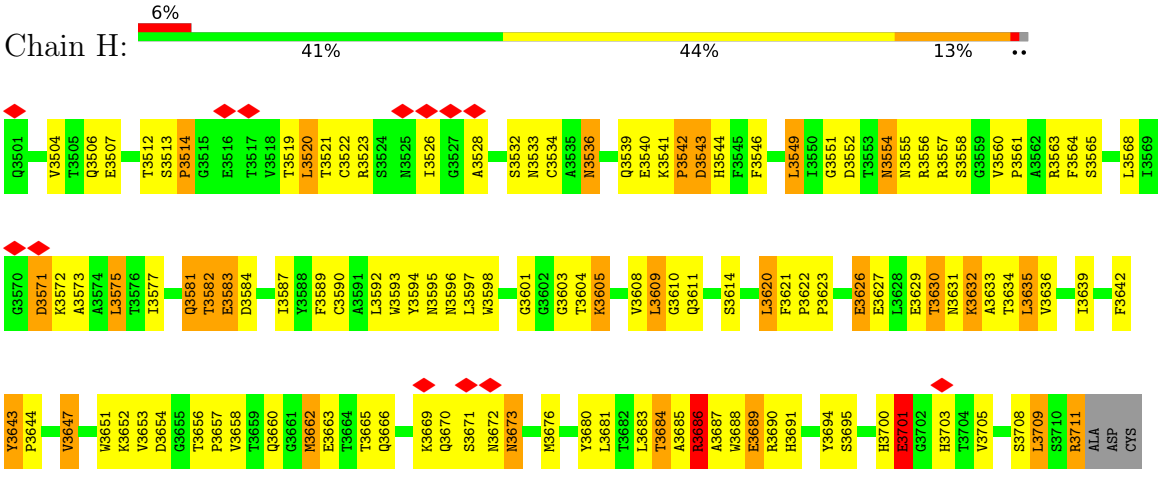
- Molecule 4: EEEV-3 antibody light chain

Chain D:



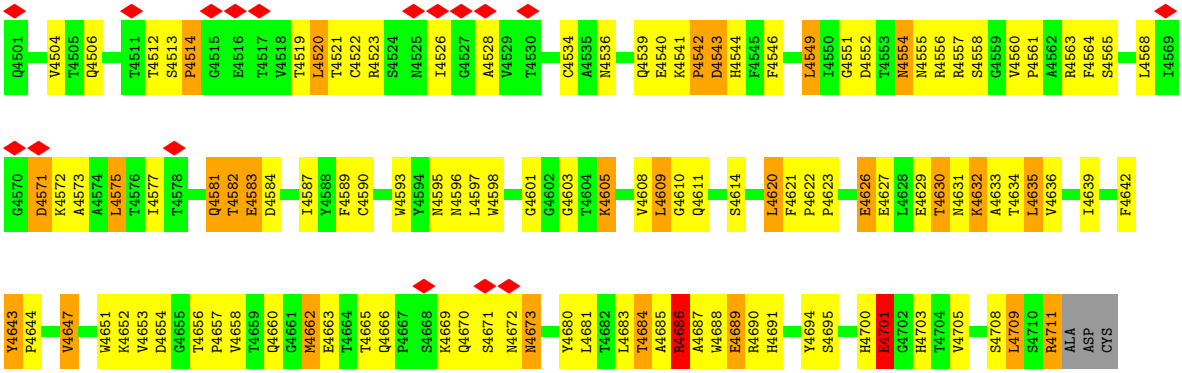
- Molecule 4: EEEV-3 antibody light chain

Chain H:



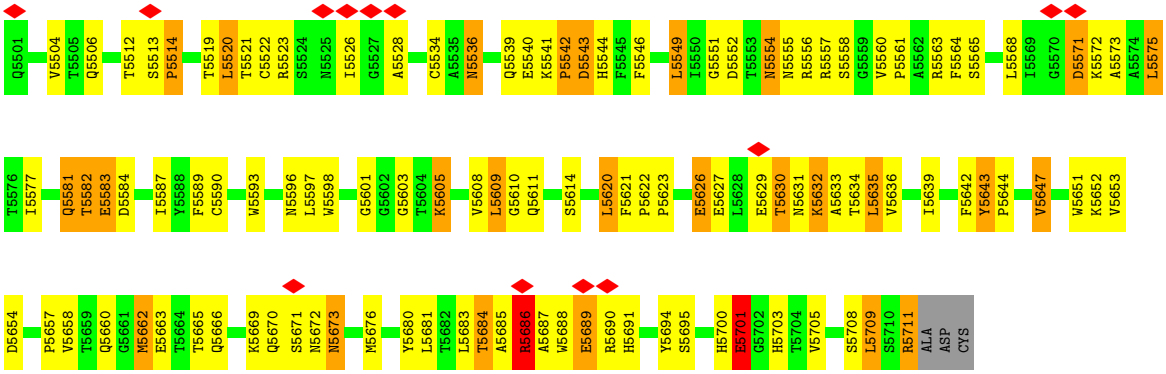
- Molecule 4: EEEV-3 antibody light chain

Chain L:



- Molecule 4: EEEV-3 antibody light chain

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8416	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 ($e^-/Å^2$)	31	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	6.783	Depositor
Minimum map value	-7.805	Depositor
Average map value	0.069	Depositor
Map value standard deviation	0.942	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	907.2, 907.2, 907.2	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.62, 1.62, 1.62	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	0.51	0/3147	0.69	1/4294 (0.0%)
1	E	0.51	0/3147	0.69	1/4294 (0.0%)
1	I	0.51	0/3147	0.69	1/4294 (0.0%)
1	M	0.51	0/3147	0.69	1/4294 (0.0%)
2	B	0.50	1/2624 (0.0%)	0.74	2/3571 (0.1%)
2	F	0.50	1/2624 (0.0%)	0.74	2/3571 (0.1%)
2	J	0.50	1/2624 (0.0%)	0.74	3/3571 (0.1%)
2	N	0.50	1/2624 (0.0%)	0.74	3/3571 (0.1%)
3	C	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	G	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	K	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
3	O	0.73	4/1714 (0.2%)	0.86	3/2340 (0.1%)
4	D	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
4	H	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
4	L	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
4	P	0.91	3/1634 (0.2%)	1.44	12/2232 (0.5%)
All	All	0.64	32/36476 (0.1%)	0.91	74/49748 (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
1	A	0	1
1	E	0	1
1	I	0	1
1	M	0	1
All	All	0	4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	5058	PRO	N-CD	17.39	1.72	1.47
3	C	58	PRO	N-CD	17.38	1.72	1.47
3	K	4058	PRO	N-CD	17.37	1.72	1.47
3	G	3058	PRO	N-CD	17.36	1.72	1.47
3	G	3041	PRO	N-CD	13.97	1.67	1.47

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	5686	ARG	NE-CZ-NH1	10.11	125.35	120.30
4	D	686	ARG	NE-CZ-NH1	10.06	125.33	120.30
4	L	4686	ARG	NE-CZ-NH1	10.00	125.30	120.30
4	H	3686	ARG	NE-CZ-NH1	9.96	125.28	120.30
4	D	635	LEU	CA-CB-CG	9.72	137.66	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	LYS	Peptide
1	E	1385	LYS	Peptide
1	I	2385	LYS	Peptide
1	M	3385	LYS	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	3063	0	2950	84	0
1	E	3063	0	2947	66	0
1	I	3063	0	2945	76	0
1	M	3063	0	2947	56	0
2	B	2550	0	2492	61	0
2	F	2550	0	2489	161	0
2	J	2550	0	2492	90	0
2	N	2550	0	2493	73	0
3	C	1671	0	1641	218	0
3	G	1671	0	1638	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1671	0	1637	224	0
3	O	1671	0	1638	224	0
4	D	1598	0	1526	193	0
4	H	1598	0	1524	286	0
4	L	1598	0	1526	202	0
4	P	1598	0	1526	191	0
All	All	35528	0	34411	1869	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 27.

The worst 5 of 1869 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:K:4032:TYR:HE1	3:K:4100:TYR:CD1	1.00	1.70
2:J:2669:SER:HA	4:L:4593:TRP:CZ3	1.21	1.65
3:C:118:ALA:HB3	3:C:150:PHE:CE2	1.17	1.64
3:G:3032:TYR:HE1	3:G:3100:TYR:CD1	1.00	1.64
3:O:5032:TYR:CE1	3:O:5100:TYR:CD1	1.86	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	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	15	54
1	E	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	15	54
1	I	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	15	54
1	M	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	15	54
2	B	323/420 (77%)	258 (80%)	65 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	323/420 (77%)	259 (80%)	64 (20%)	0	100	100
2	J	323/420 (77%)	259 (80%)	64 (20%)	0	100	100
2	N	323/420 (77%)	259 (80%)	64 (20%)	0	100	100
3	C	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	6	34
3	G	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	6	34
3	K	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	6	34
3	O	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	6	34
4	D	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	15	54
4	H	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	15	54
4	L	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	15	54
4	P	209/214 (98%)	187 (90%)	20 (10%)	2 (1%)	15	54
All	All	4584/5172 (89%)	3858 (84%)	682 (15%)	44 (1%)	20	54

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASP
3	C	43	LYS
4	D	543	ASP
1	E	1390	ASP
3	G	3043	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	339/370 (92%)	334 (98%)	5 (2%)	65	80
1	E	339/370 (92%)	334 (98%)	5 (2%)	65	80
1	I	339/370 (92%)	334 (98%)	5 (2%)	65	80
1	M	339/370 (92%)	334 (98%)	5 (2%)	65	80
2	B	282/367 (77%)	279 (99%)	3 (1%)	73	84

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	282/367 (77%)	279 (99%)	3 (1%)	73	84
2	J	282/367 (77%)	279 (99%)	3 (1%)	73	84
2	N	282/367 (77%)	279 (99%)	3 (1%)	73	84
3	C	188/188 (100%)	178 (95%)	10 (5%)	22	47
3	G	188/188 (100%)	178 (95%)	10 (5%)	22	47
3	K	188/188 (100%)	178 (95%)	10 (5%)	22	47
3	O	188/188 (100%)	178 (95%)	10 (5%)	22	47
4	D	178/183 (97%)	149 (84%)	29 (16%)	2	13
4	H	178/183 (97%)	149 (84%)	29 (16%)	2	13
4	L	178/183 (97%)	149 (84%)	29 (16%)	2	13
4	P	178/183 (97%)	149 (84%)	29 (16%)	2	13
All	All	3948/4432 (89%)	3760 (95%)	188 (5%)	29	50

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	4554	ASN
1	M	3217	ASN
4	L	4582	THR
4	L	4662	MET
3	O	5005	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	3581	GLN
3	O	5084	ASN
2	J	2825	GLN
3	O	5082	GLN
4	P	5581	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

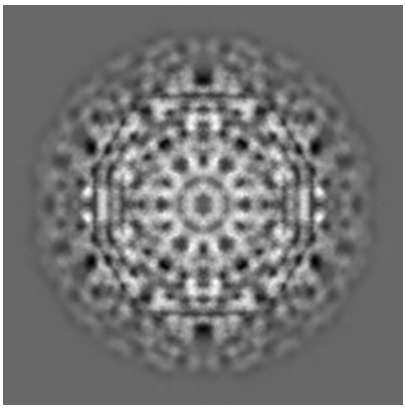
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9274. These allow visual inspection of the internal detail of the map and identification of artifacts.

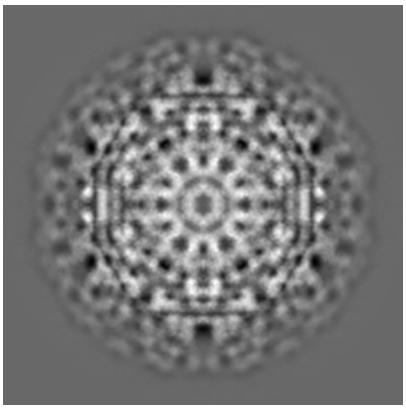
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

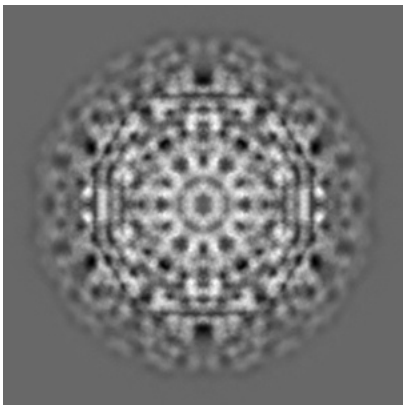
6.1.1 Primary map



X

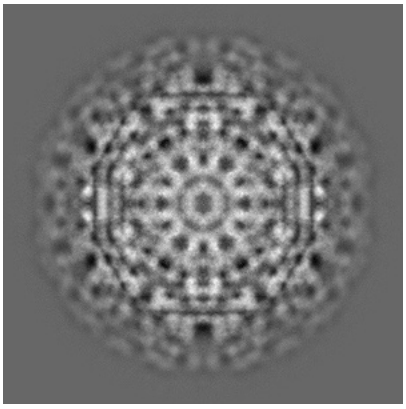


Y

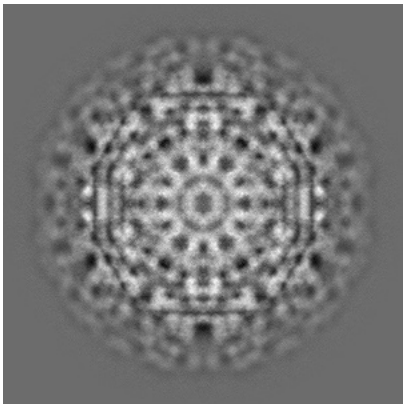


Z

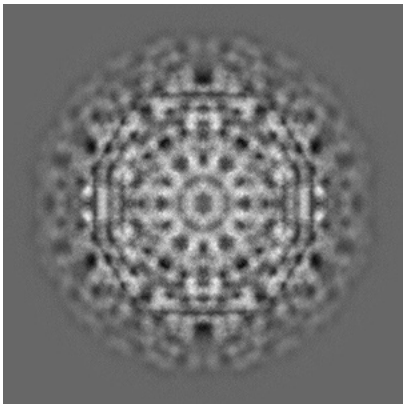
6.1.2 Raw map



X



Y

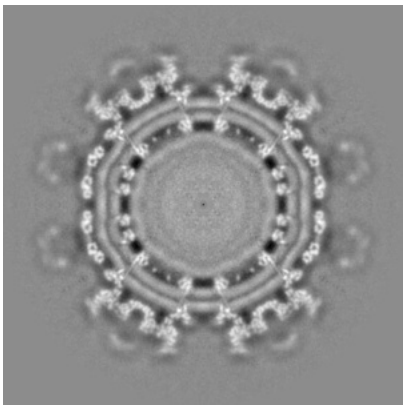


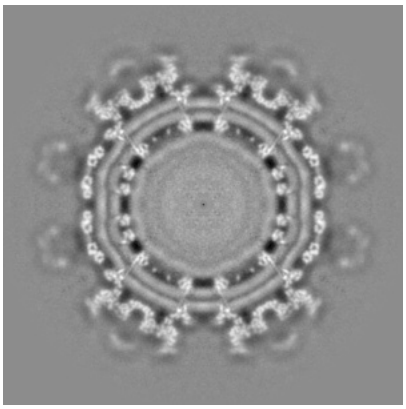
Z

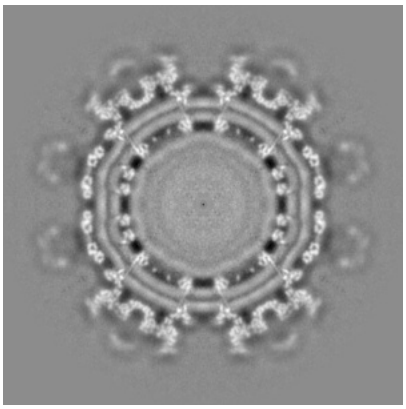
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

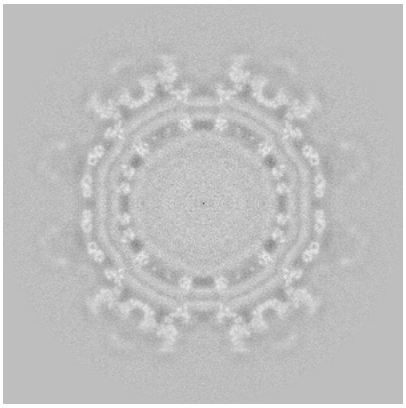
6.2.1 Primary map

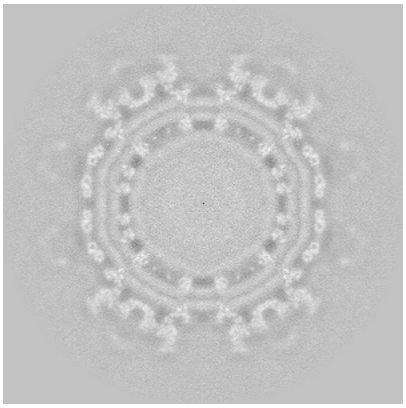

X Index: 280

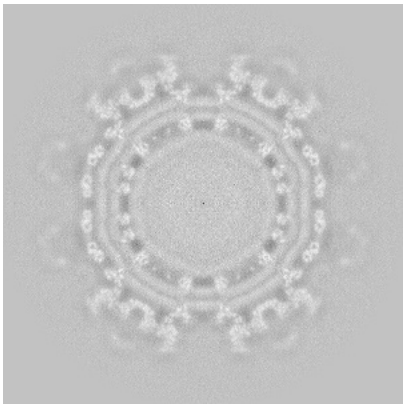

Y Index: 280


Z Index: 280

6.2.2 Raw map


X Index: 280

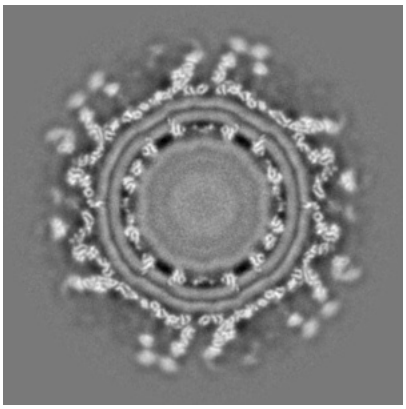

Y Index: 280


Z Index: 280

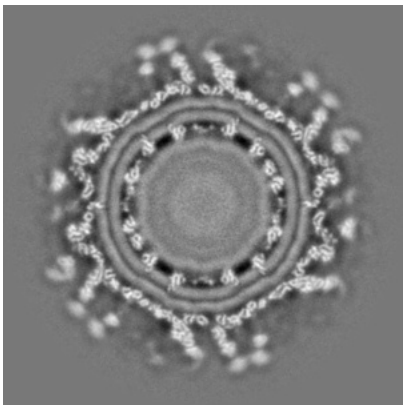
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

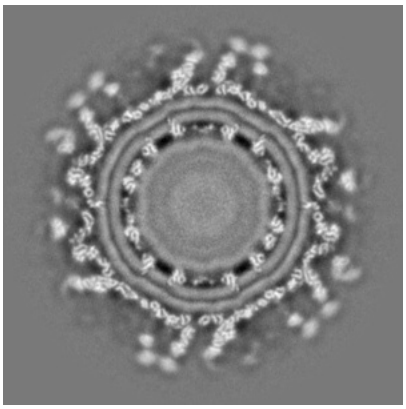
6.3.1 Primary map



X Index: 245

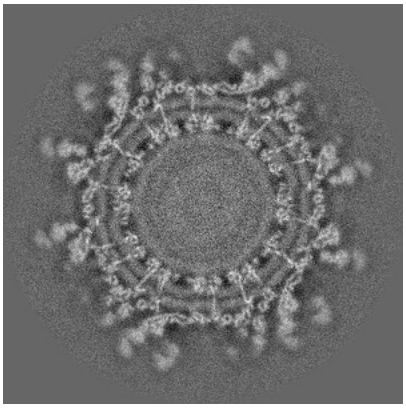


Y Index: 315

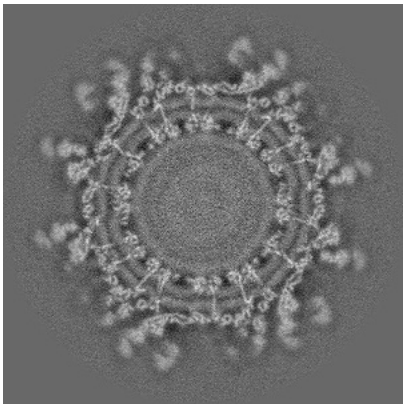


Z Index: 245

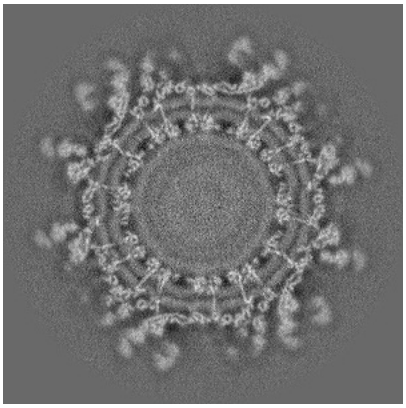
6.3.2 Raw map



X Index: 298



Y Index: 298



Z Index: 298

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

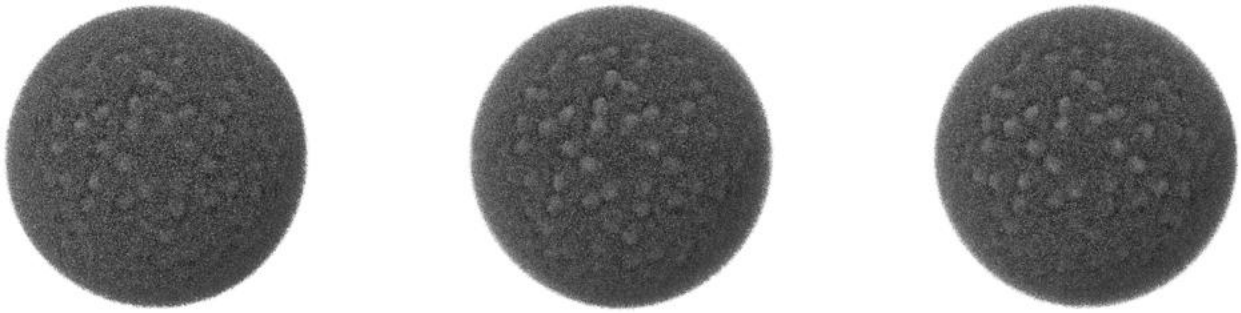
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

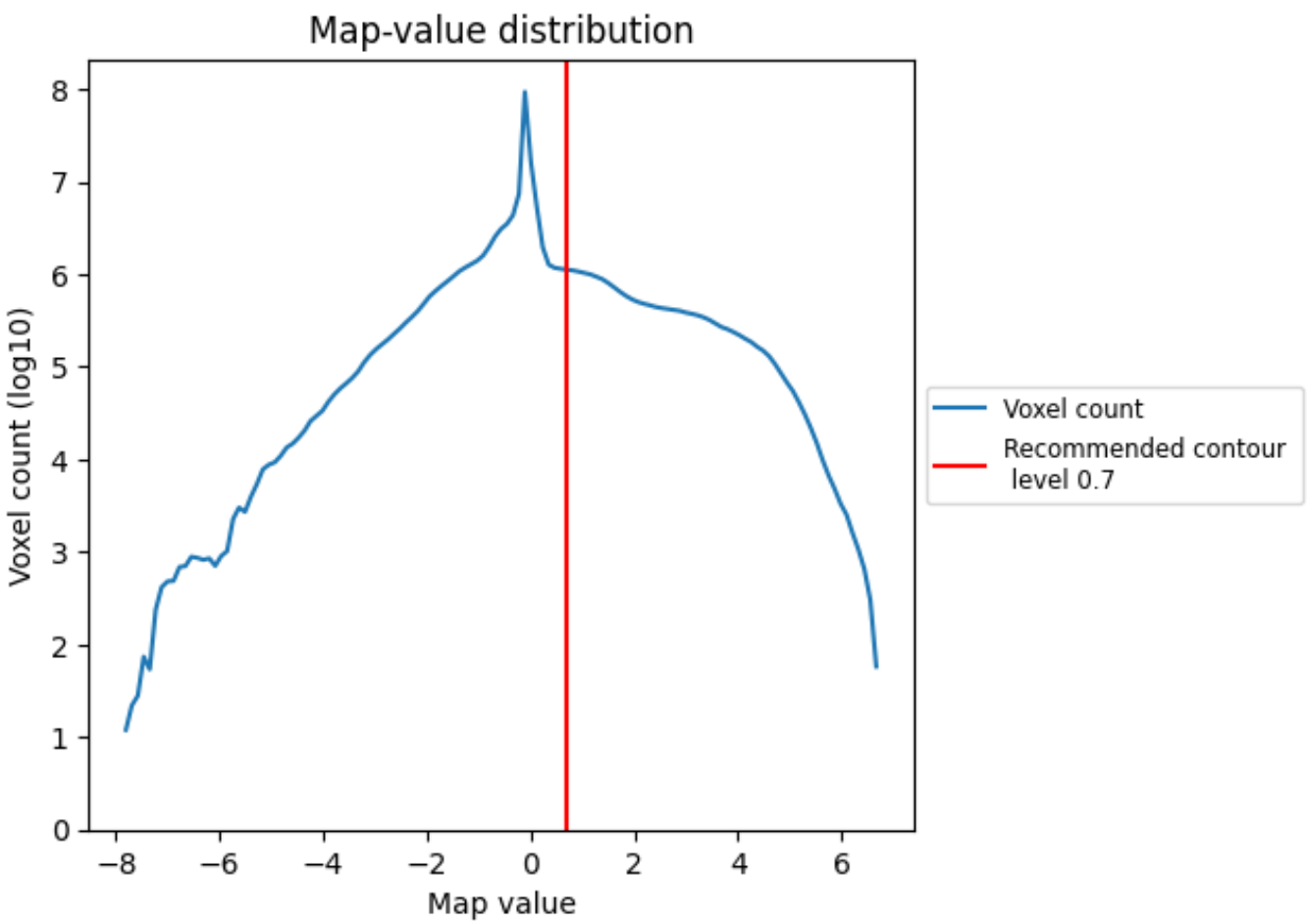
6.5 Mask visualisation (i)

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

7 Map analysis (i)

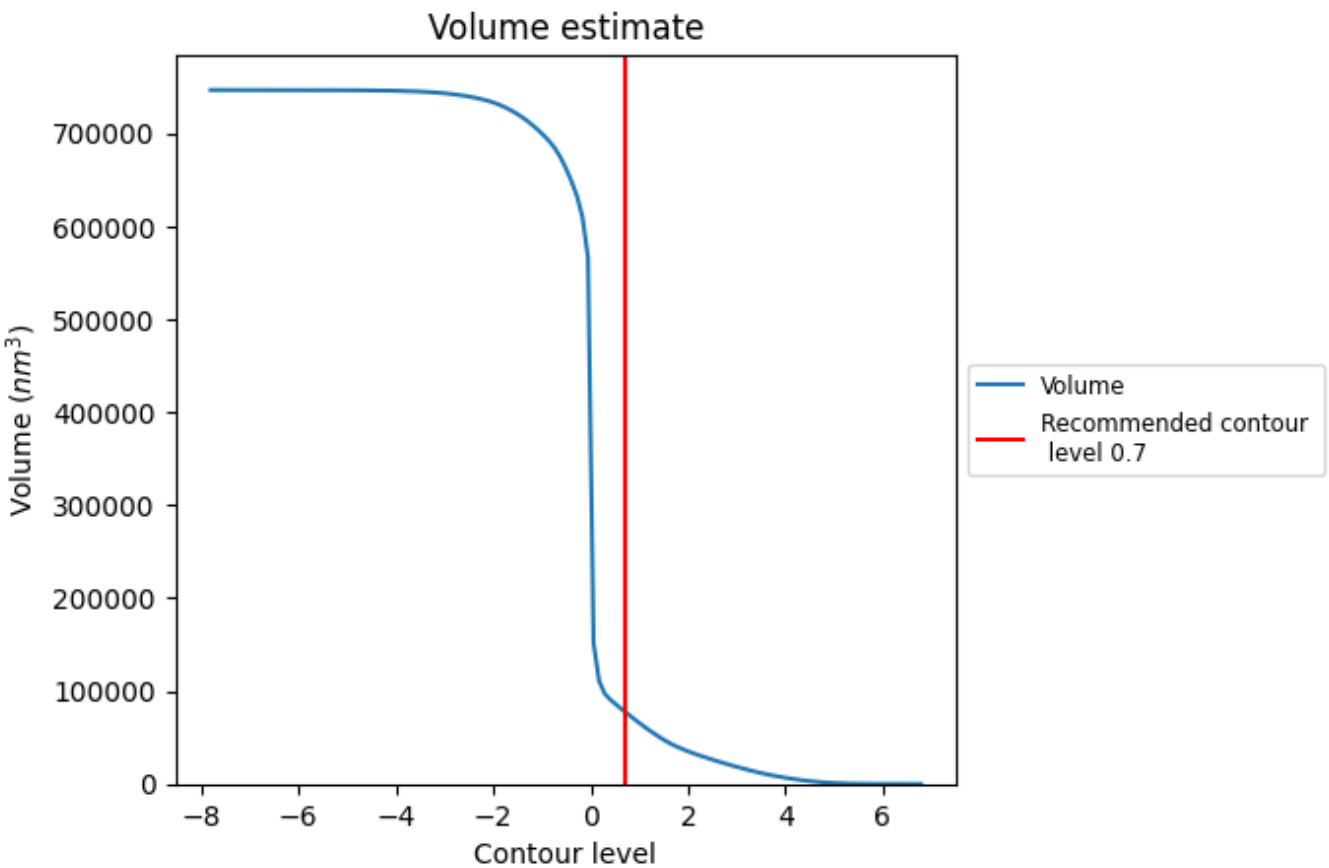
This section contains the results of statistical analysis of the map.

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.

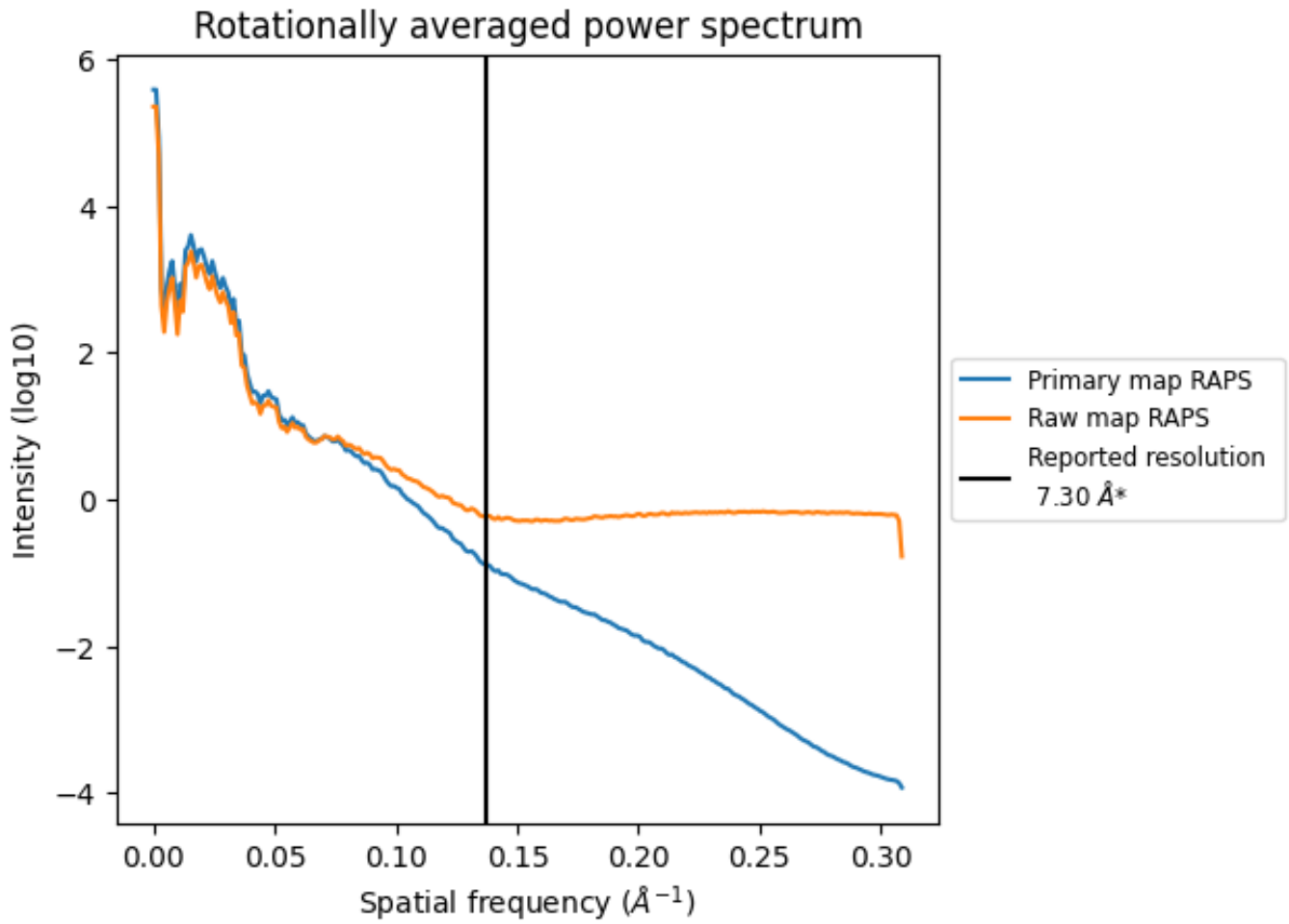
7.2 Volume estimate (i)



The volume at the recommended contour level is 77807 nm^3; this corresponds to an approximate mass of 70285 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)

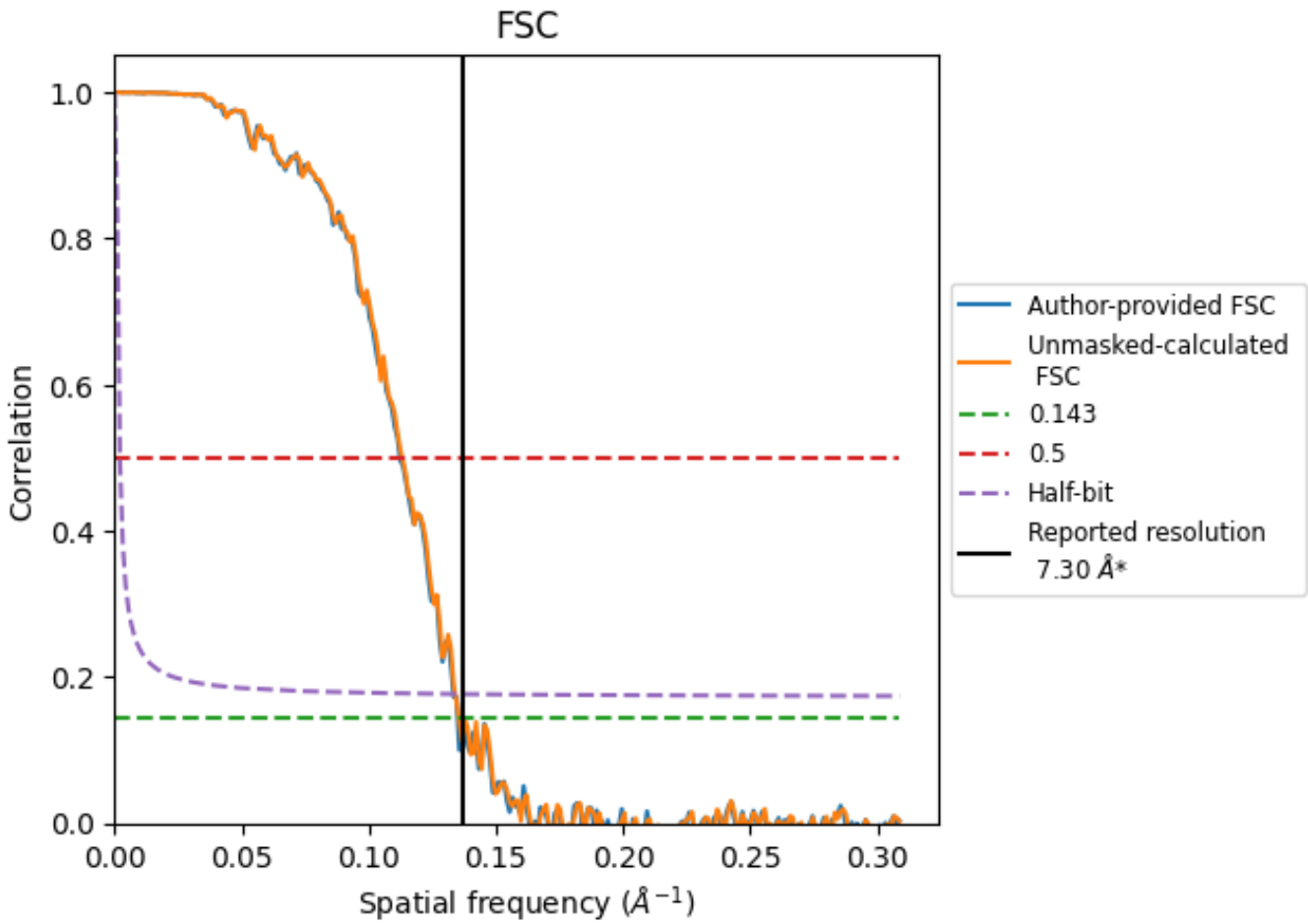


*Reported resolution corresponds to spatial frequency of 0.137 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.137 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	7.41	8.90	7.50
Unmasked-calculated*	7.39	8.83	7.46

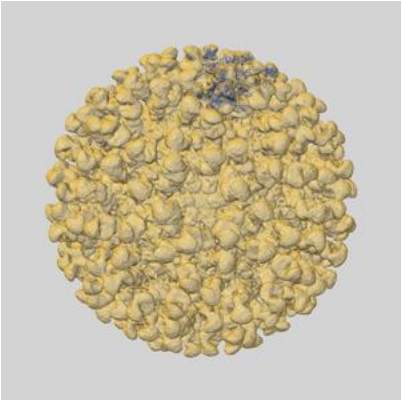
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

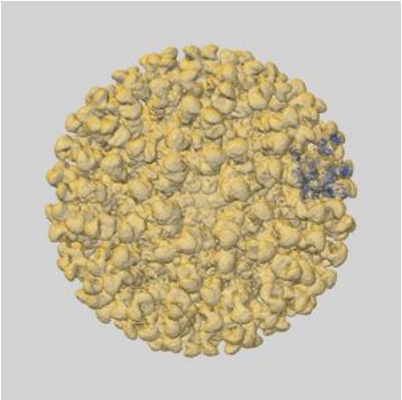
This section contains information regarding the fit between EMDB map EMD-9274 and PDB model 6MW9. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

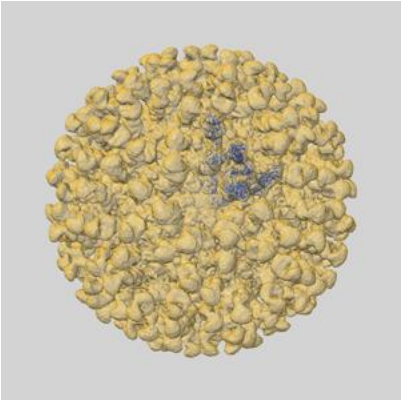
9.1.1 Map-model overlay (i)



X

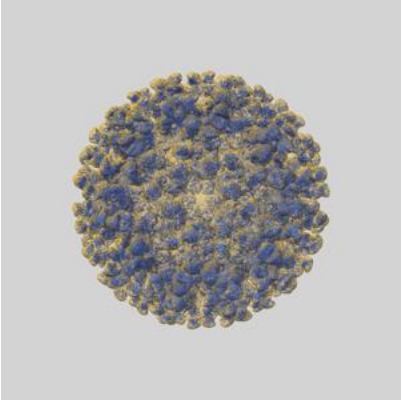


Y

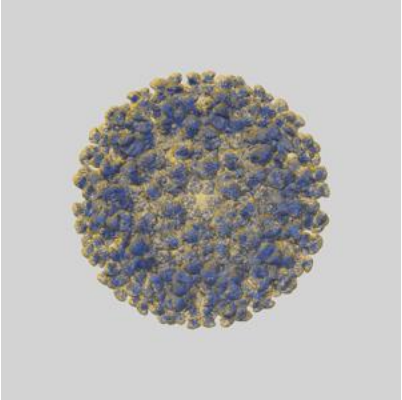


Z

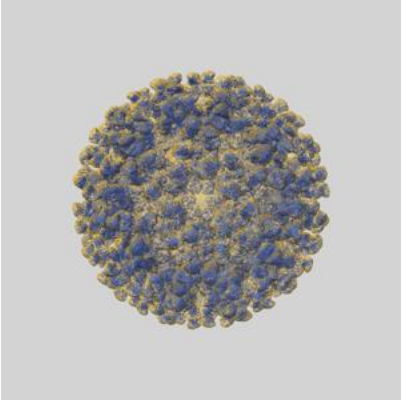
9.1.2 Map-model assembly overlay (i)



X



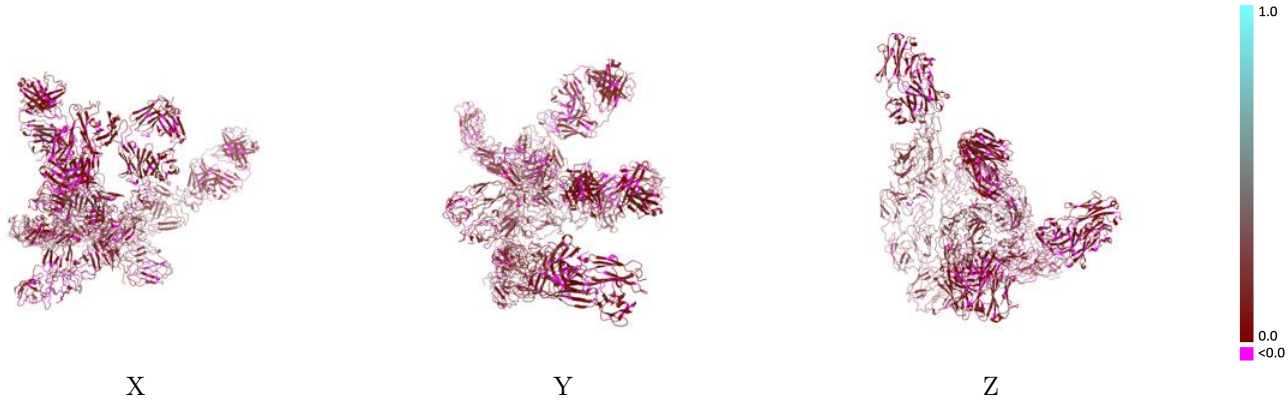
Y



Z

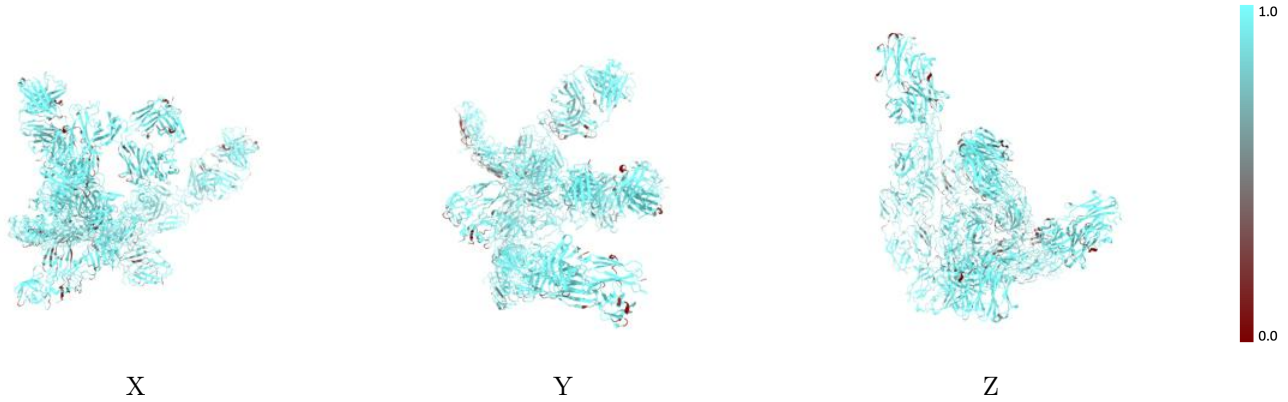
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



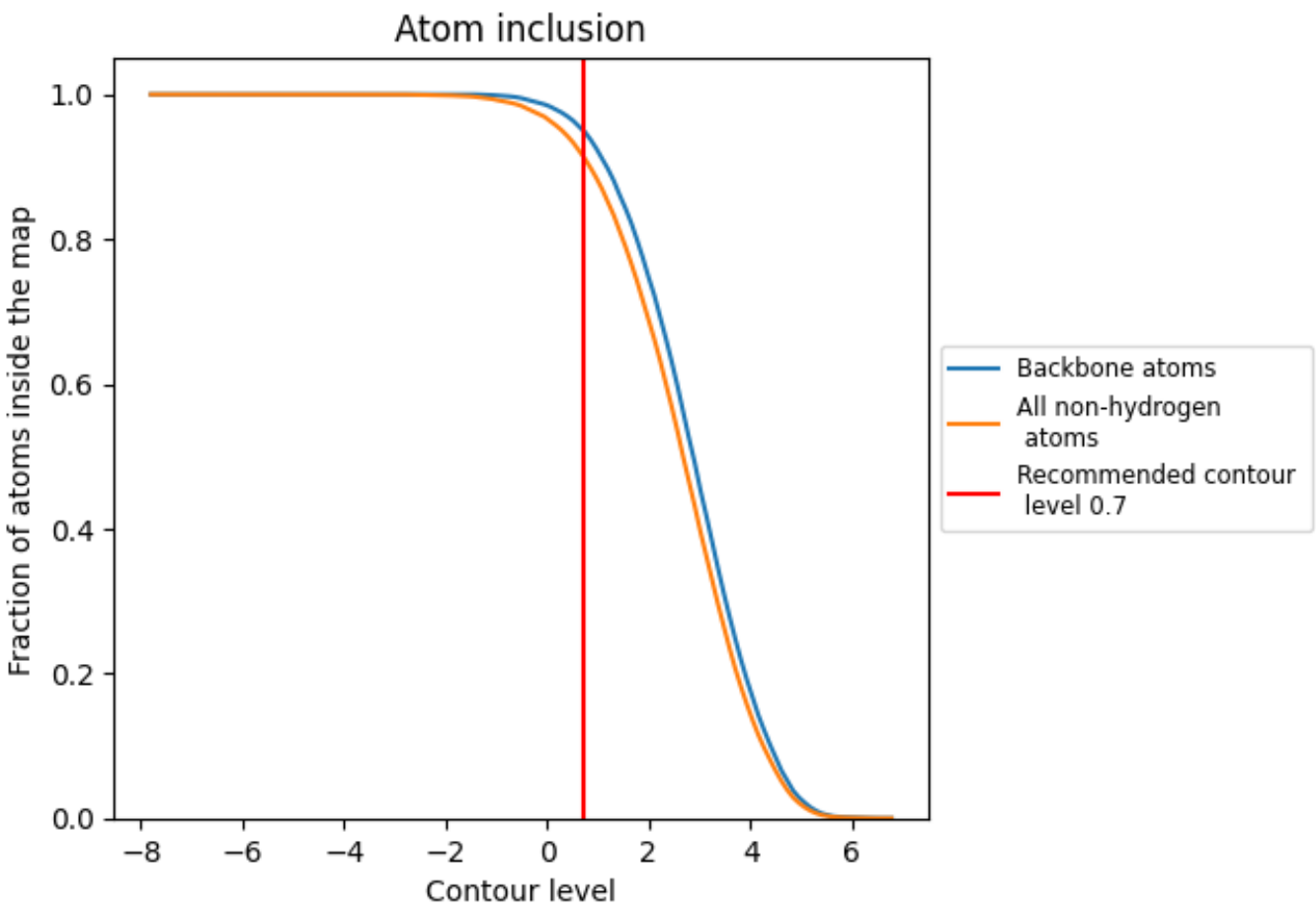
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9148	0.0970
A	0.9265	0.1300
B	0.9347	0.1420
C	0.9361	0.0660
D	0.8932	0.0810
E	0.8917	0.1160
F	0.9335	0.1220
G	0.9337	0.0780
H	0.9186	0.0640
I	0.9245	0.1170
J	0.9299	0.0970
K	0.9239	0.0520
L	0.8951	0.0590
M	0.8758	0.0940
N	0.8974	0.0920
O	0.9270	0.0720
P	0.9091	0.0750