wwPDB EM Validation Summary Report

Aug 9, 2026 – 04:22 PM JST

PDB ID	:	23SG / pdb_000023sg
EMDB ID	:	EMD-69208
Title	:	The composite Cryo-EM structure of bacteriophage RAN69 pre-ejectosome-portal complex
Authors	:	Ruan, Z.; Hu, H.; Wang, A.; Shao, Q.; Li, X.; Xie, L.; Sun, Z.; Yu, J.; Fang, Q.
Deposited on	:	2026-02-15
Resolution	:	3.00 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:

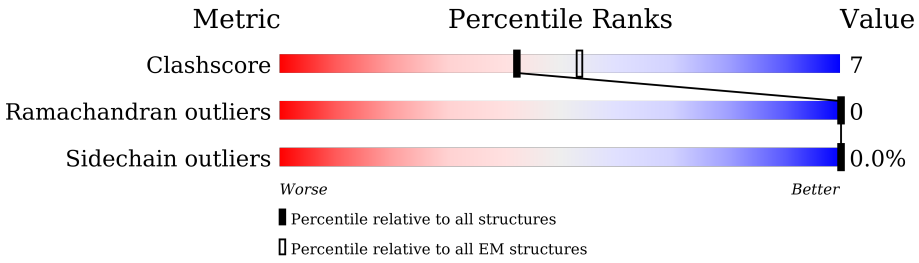
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

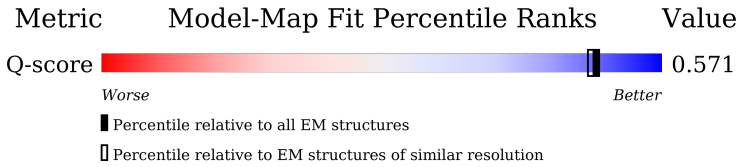
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	G	893	9% 77% 13% 10%
1	N	893	7% 78% 12% 10%
2	X	195	28% 67% 8% 25%
2	a	195	27% 61% 11% 28%

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Mol	Chain	Length	Quality of chain
3	S	1239	18% 71% 21% 8%
4	A	531	13% 78% 15% 7%
4	D	531	14% 73% 19% 7%
4	d	531	11% 79% 16% 6%
5	g	87	14% 36% 6% 59%
5	m	87	11% 38% 59%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 35335 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 gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	806	Total	C	N	O	S	0	0
			6173	3795	1105	1248	25		
1	G	807	Total	C	N	O	S	0	0
			6179	3800	1108	1246	25		

- Molecule 2 is a protein called gp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	146	Total	C	N	O	S	0	0
			1109	688	198	218	5		
2	a	140	Total	C	N	O	S	0	0
			1079	669	191	213	6		

- Molecule 3 is a protein called gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	1135	Total	C	N	O	S	0	0
			8748	5443	1580	1678	47		

- Molecule 4 is a protein called portal gp19.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	501	Total	C	N	O	S	0	0
			3883	2442	655	779	7		
4	A	492	Total	C	N	O	S	0	0
			3822	2407	643	765	7		
4	D	492	Total	C	N	O	S	0	0
			3822	2407	643	765	7		

- Molecule 5 is a protein called gp20.

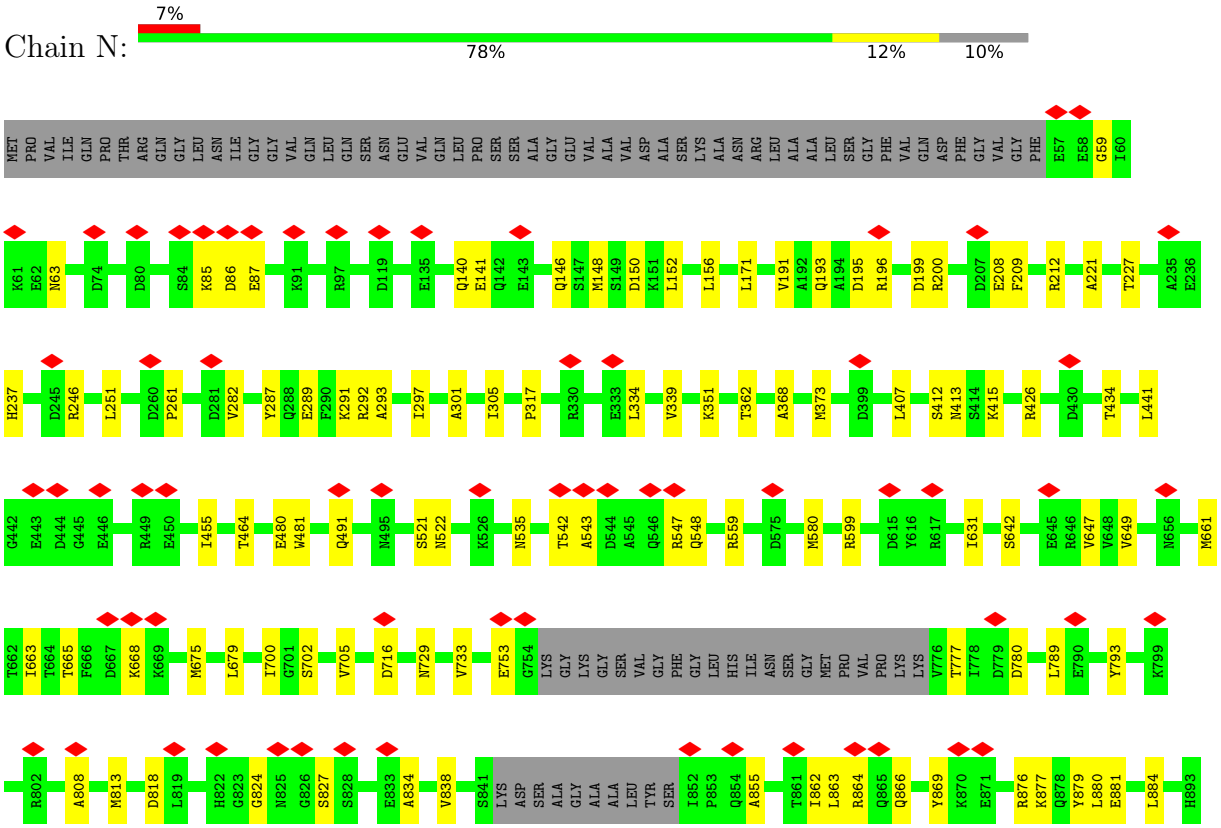
Mol	Chain	Residues	Atoms					AltConf	Trace
5	m	36	Total	C	N	O	S	0	0
			260	160	50	49	1		
5	g	36	Total	C	N	O	S	0	0
			260	160	50	49	1		

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.

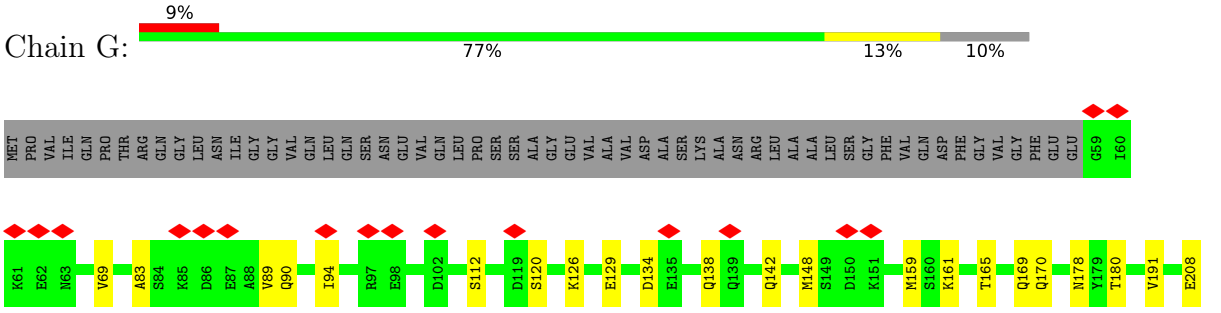
• Molecule 1: gp11

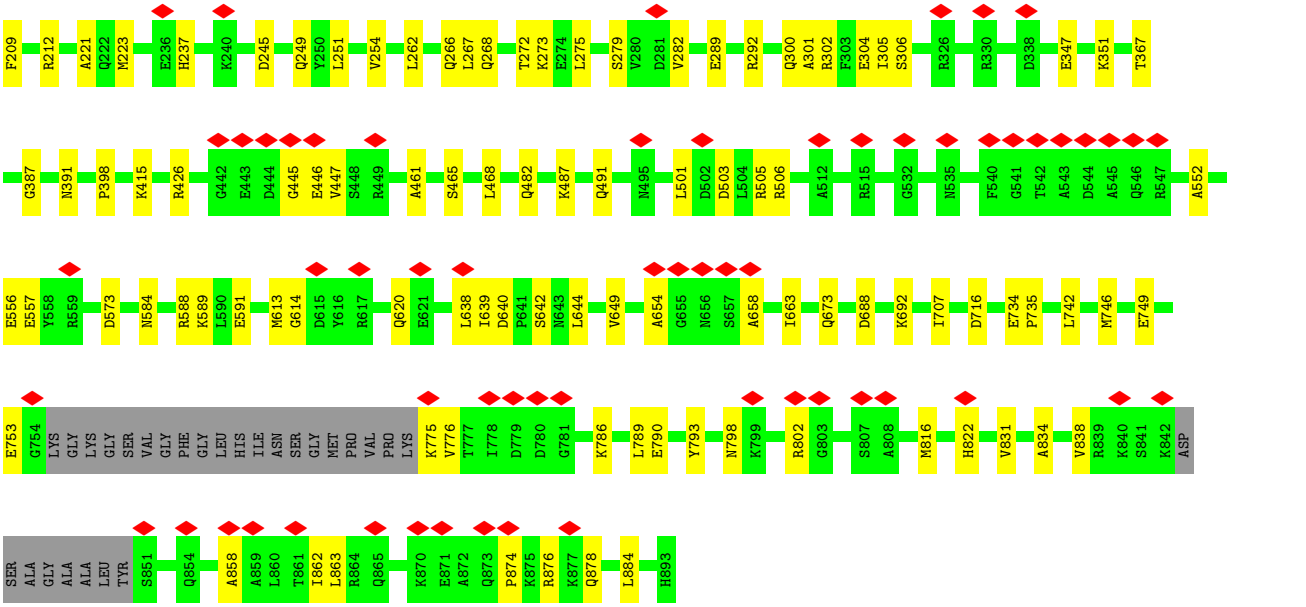
Chain N:



• Molecule 1: gp11

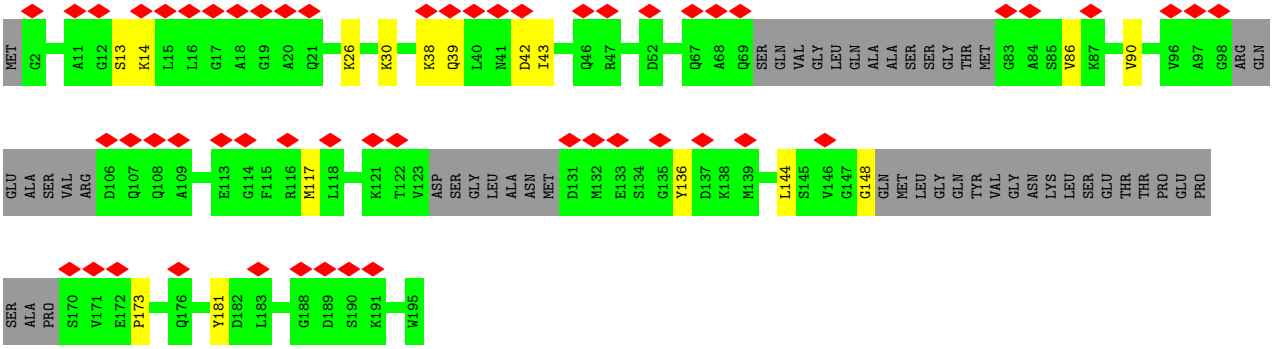
Chain G:





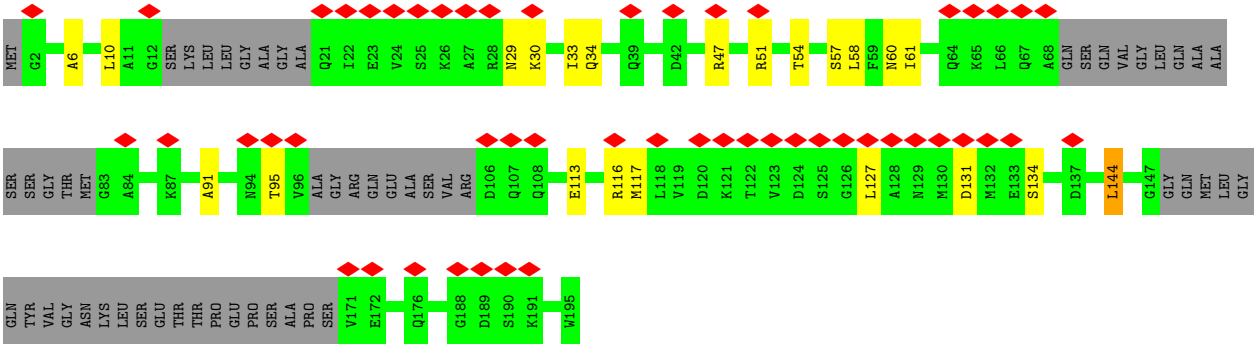
• Molecule 2: gp12





• Molecule 2: gp12

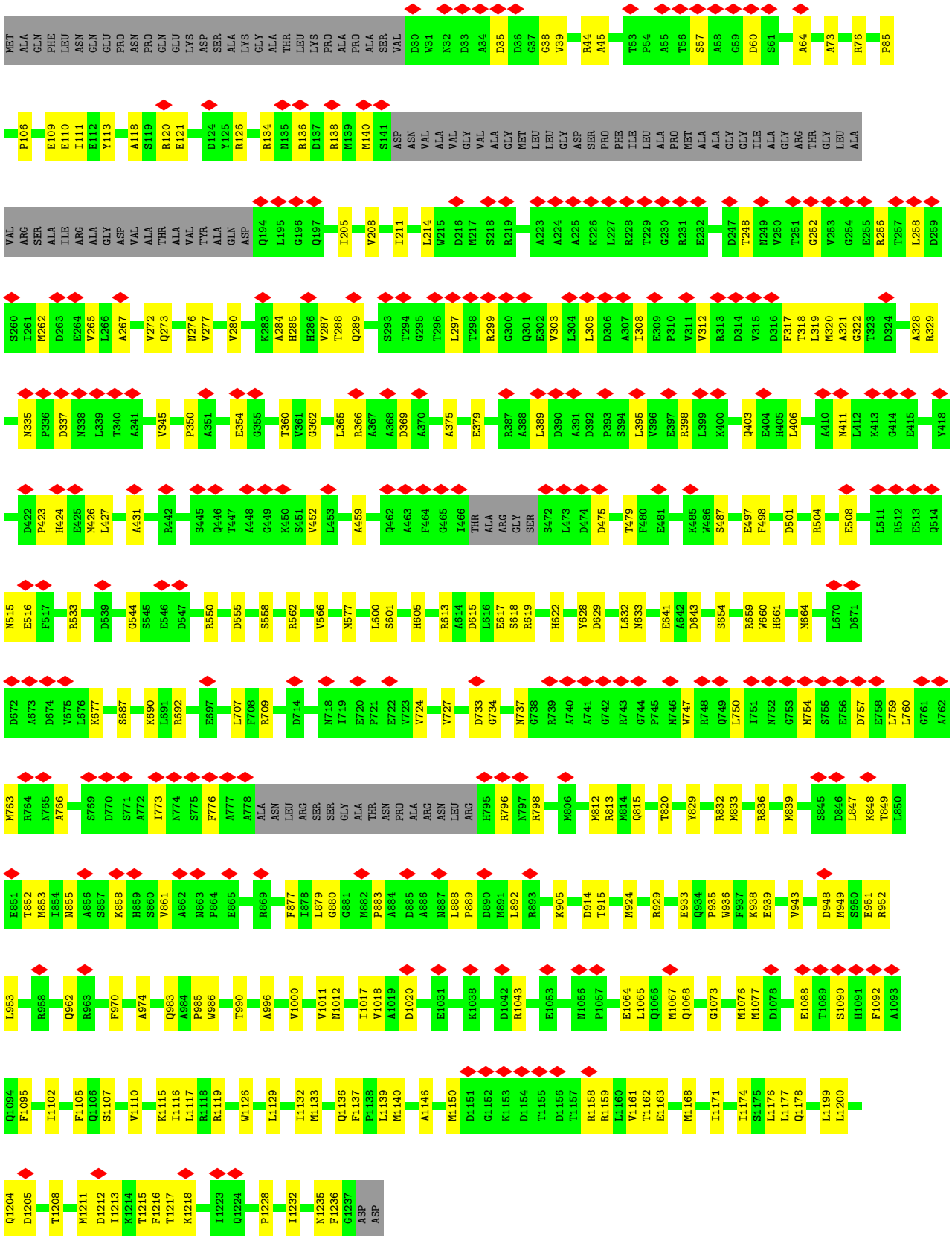




• Molecule 3: gp10

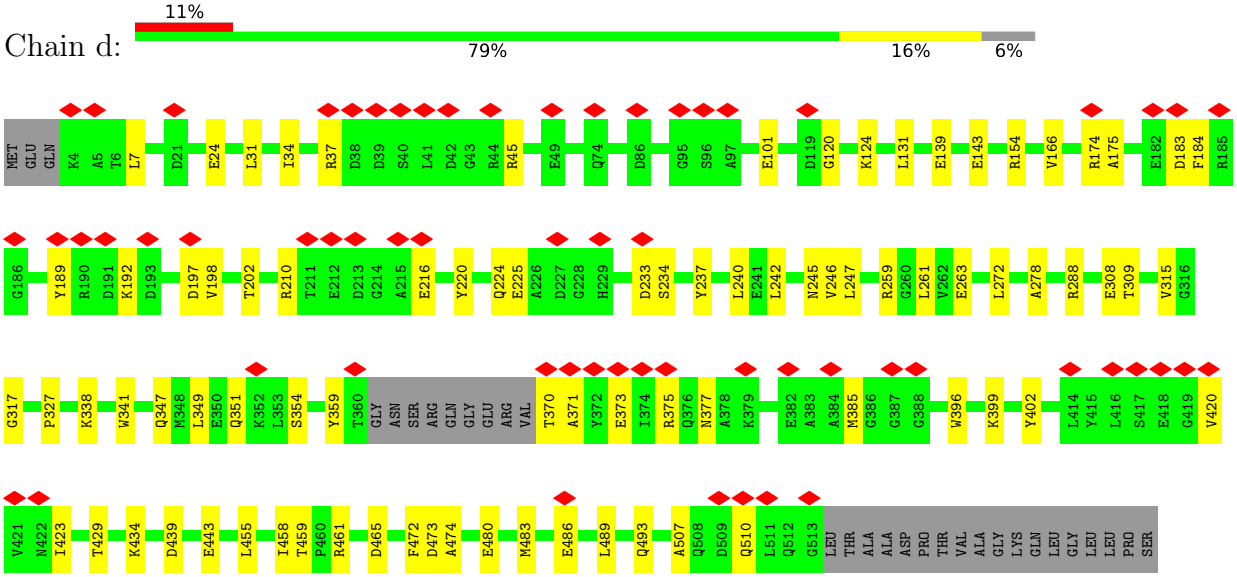
Chain S:


18%
71%
21%
8%


MET ALA GLN PHE LEU ASN GLN GLU PRO ASN PRO GLN GLU LYS ASP SER ALA LYS GLY ALA THR LEU LYS PRO ALA PRO ALA SER VAL D30 W31 N32 D33 A34 D35 D36 G37 G38 V39 R44 A45 T53 P54 A55 T56 S57 A58 G59 D60 S61 A64 A73 R76 P85
P106 E109 E110 I111 E112 Y113 A118 S119 R120 E121 D124 Y125 R126 R134 N135 R136 D137 R138 M139 M140 S141 ASP ASN VAL ALA VAL GLY VAL ALA GLY MET LEU LEU GLY ASP SER PRO PHE ILE LEU ALA PRO MET ALA ALA GLY GLY ILE ALA GLY ARG THR GLY LEU ALA
VAL ARG SER ALA ILE ARG ALA GLY ASP VAL ALA ALA THR ALA VAL TYR ALA GLN ASP Q194 L195 G196 Q197 I205 V208 I211 L214 W215 D216 M217 S218 R219 A223 A224 A225 K226 L227 R228 T229 G230 R231 E232 D247 T248 N249 V250 T251 G252 V253 G254 E255 R256 T257 L258 D259
S260 I261 M262 D263 E264 V265 L266 A267 V272 Q273 N276 V277 V280 K283 A284 H285 H286 V287 T288 Q289 S293 T294 G295 T296 L297 T298 R299 G300 Q301 E302 V303 L304 L305 D306 A307 I308 E309 P310 V311 V312 R313 D314 V315 D316 F317 T318 L319 M320 A321 G322 T323 D324 A328 R329
N335 P336 D337 N338 L339 T340 A341 V345 P350 A351 E354 G355 T360 V361 G362 L365 R366 A367 A368 D369 A370 A375 E379 R387 A388 L389 D390 A391 D392 P393 S394 L395 V396 E397 R398 L399 K400 Q403 E404 H405 L406 A410 N411 L412 K413 G414 E415 Y418
D422 P423 H424 E425 M426 L427 A431 R442 S445 Q446 T447 A448 G449 K450 S451 V452 L453 A459 Q462 A463 F464 G465 I466 THR ALA ARG GLY SER S472 L473 D474 D475 T479 F480 E481 K485 W486 S487 E497 F498 D501 R504 E508 L511 R512 E513 Q514
N515 E516 F517 R533 D539 G544 S545 E546 D547 R550 D555 S558 R562 V566 M577 L600 S601 H605 R613 A614 D615 L616 E617 S618 R619 H622 Y628 D629 L632 N633 E641 A642 D643 S654 R659 W660 H661 M664 L670 D671
D672 A673 D674 V675 L676 K677 S687 K690 L691 R692 E697 L707 F708 R709 D714 N718 I719 E720 P721 E722 V723 V724 V727 D733 G734 N737 G738 R739 A740 A741 G742 R743 G744 P745 M746 W747 R748 Q749 L750 I751 N752 G753 M754 S755 E756 D757 E758 L759 L760 G761 A762
W763 R764 N765 A766 S769 D770 S771 A772 I773 W774 S775 F776 A777 A778 ALA ASN LEU ARG SER SER GLY ALA THR ASN PRO ALA ARG ASN LEU ARG H795 R796 N797 R798 M806 M812 R813 M814 Q815 T820 Y829 R832 M833 R836 M839 S845 D846 L847 K848 T849 L850
E851 T852 M853 I854 N855 A856 S857 K858 H859 S860 V861 A862 N863 P864 E865 R869 F877 I878 L879 G880 G881 M882 P883 A884 D885 A886 N887 L888 P889 D890 M891 L892 R893 K905 D914 T915 M924 R929 E933 Q934 P935 W936 F937 K938 E939 V943 D948 M949 S950 E951 R952
L953 R958 Q962 R963 F970 A974 Q983 A984 P985 W986 T990 A996 V1000 V1011 N1012 I1017 V1018 A1019 D1020 E1031 K1038 D1042 R1043 E1053 N1056 P1057 E1064 L1065 Q1066 M1067 Q1068 G1073 M1076 M1077 D1078 E1088 T1089 S1090 H1091 F1092 A1093
Q1094 F1095 I1102 F1105 Q1106 S1107 V1110 K1115 I1116 L1117 R1118 R1119 W1126 L1129 I1132 M1133 Q1136 F1137 P1138 L1139 M1140 A1146 M1150 D1151 G1152 K1153 D1154 T1155 D1156 T1157 R1158 R1159 L1160 V1161 T1162 E1163 M1168 I1171 I1174 S1175 L1176 L1177 Q1178 L1199 L1200
Q1204 D1205 T1208 M1211 D1212 I1213 K1214 T1215 F1216 T1217 K1218 I1223 Q1224 P1228 I1232 N1235 F1236 G1237 ASP ASP

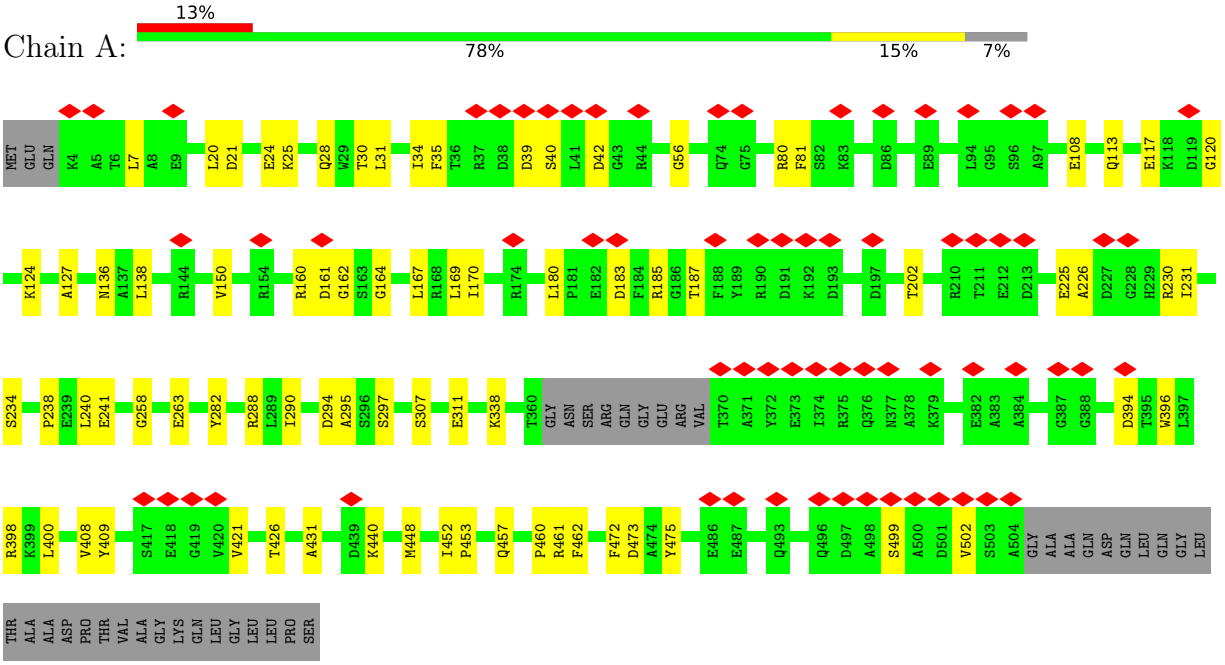
• Molecule 4: portal gp19

Chain d:



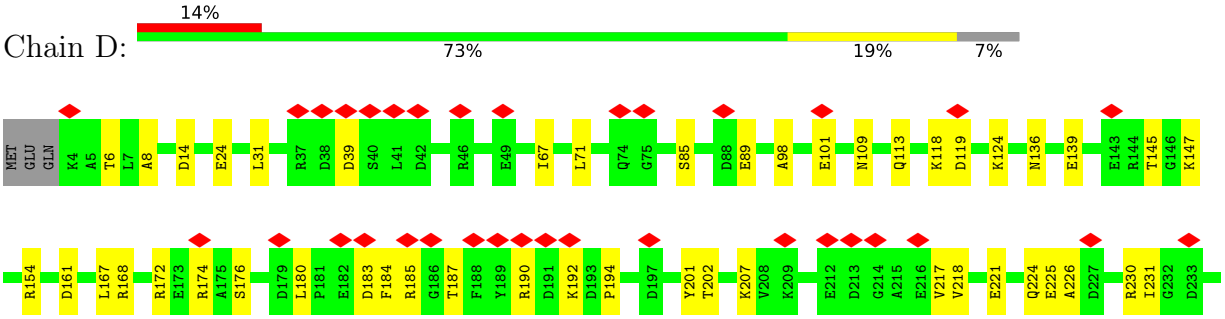
• Molecule 4: portal gp19

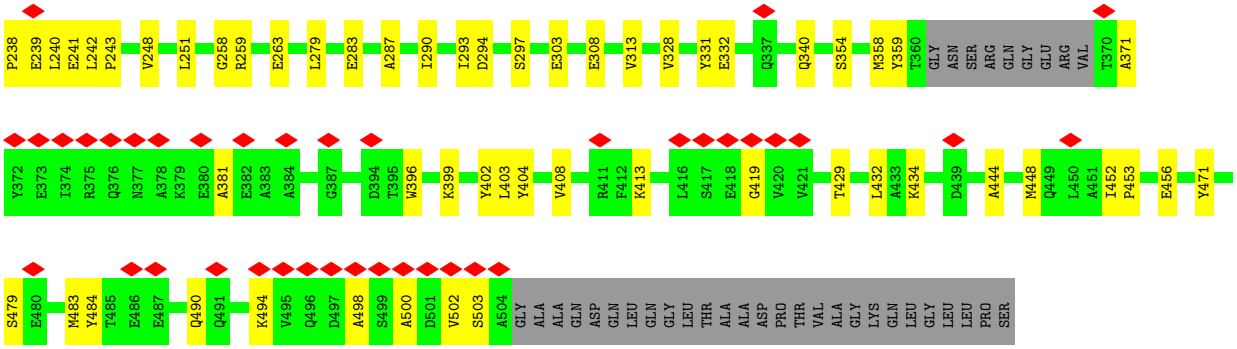
Chain A:



• Molecule 4: portal gp19

Chain D:

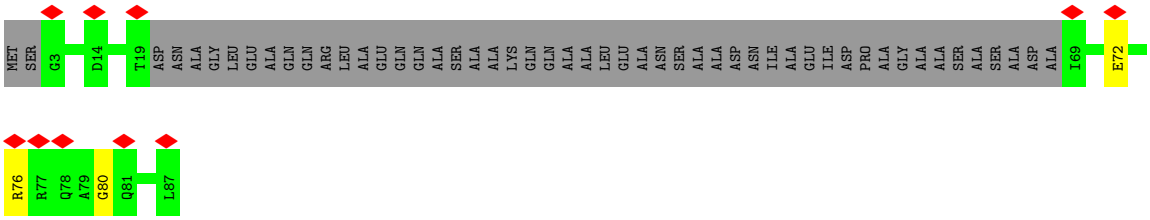




- Molecule 5: gp20

Chain m:

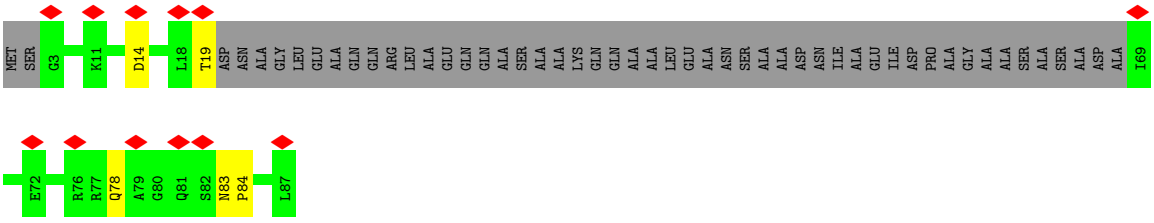




- Molecule 5: gp20

Chain g:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25878	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	13.135	Depositor
Minimum map value	-7.616	Depositor
Average map value	-0.061	Depositor
Map value standard deviation	0.983	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	342.72003, 342.72003, 342.72003	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	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	G	0.12	0/6264	0.26	0/8454
1	N	0.14	0/6258	0.27	0/8448
2	X	0.23	0/1120	0.39	0/1504
2	a	0.24	0/1090	0.42	0/1465
3	S	0.12	0/8896	0.27	0/12028
4	A	0.11	0/3888	0.27	0/5263
4	D	0.11	0/3888	0.26	0/5263
4	d	0.12	0/3949	0.28	0/5345
5	g	0.11	0/259	0.31	0/341
5	m	0.11	0/259	0.33	0/341
All	All	0.13	0/35871	0.28	0/48452

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

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	G	6179	0	6059	76	0
1	N	6173	0	6040	71	0
2	X	1109	0	1091	11	0
2	a	1079	0	1054	20	0
3	S	8748	0	8636	160	0
4	A	3822	0	3737	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3822	0	3737	64	0
4	d	3883	0	3792	59	0
5	g	260	0	282	7	0
5	m	260	0	282	2	0
All	All	35335	0	34710	472	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 7.

The worst 5 of 472 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:S:403:GLN:NE2	3:S:426:MET:SD	2.51	0.82
3:S:35:ASP:OD2	3:S:659:ARG:NH1	2.20	0.75
3:S:747:TRP:HE3	3:S:847:LEU:HD23	1.52	0.74
3:S:855:ASN:HA	3:S:858:LYS:HE3	1.69	0.74
3:S:1129:LEU:HA	3:S:1132:ILE:HD12	1.69	0.73

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	G	801/893 (90%)	794 (99%)	7 (1%)	0	100	100
1	N	800/893 (90%)	792 (99%)	8 (1%)	0	100	100
2	X	136/195 (70%)	131 (96%)	5 (4%)	0	100	100
2	a	130/195 (67%)	126 (97%)	4 (3%)	0	100	100
3	S	1127/1239 (91%)	1102 (98%)	25 (2%)	0	100	100
4	A	488/531 (92%)	477 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	488/531 (92%)	477 (98%)	11 (2%)	0	100	100
4	d	497/531 (94%)	487 (98%)	10 (2%)	0	100	100
5	g	32/87 (37%)	32 (100%)	0	0	100	100
5	m	32/87 (37%)	32 (100%)	0	0	100	100
All	All	4531/5182 (87%)	4450 (98%)	81 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	G	650/714 (91%)	650 (100%)	0	100	100
1	N	649/714 (91%)	649 (100%)	0	100	100
2	X	114/153 (74%)	114 (100%)	0	100	100
2	a	113/153 (74%)	112 (99%)	1 (1%)	70	85
3	S	906/978 (93%)	906 (100%)	0	100	100
4	A	403/431 (94%)	403 (100%)	0	100	100
4	D	403/431 (94%)	403 (100%)	0	100	100
4	d	408/431 (95%)	408 (100%)	0	100	100
5	g	27/58 (47%)	27 (100%)	0	100	100
5	m	27/58 (47%)	27 (100%)	0	100	100
All	All	3700/4121 (90%)	3699 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	451	ASN
4	A	422	ASN
1	G	584	ASN
1	G	744	ASN
4	A	493	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

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.

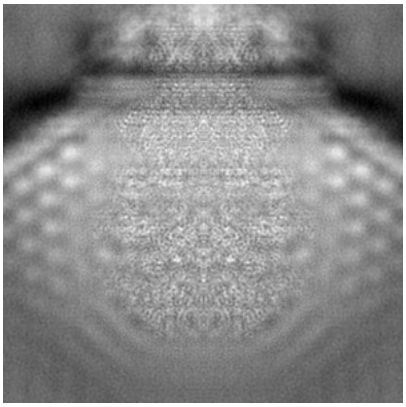
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-69208. These allow visual inspection of the internal detail of the map and identification of artifacts.

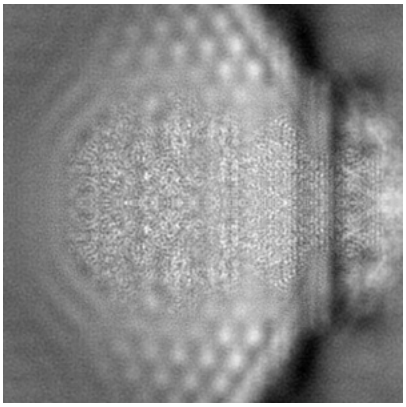
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

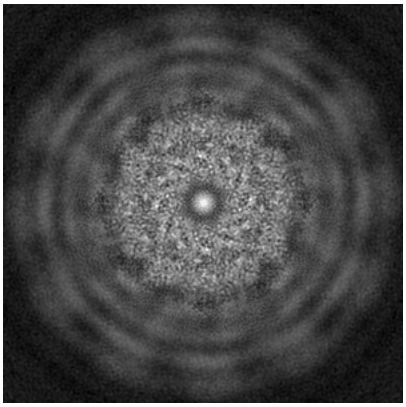
6.1.1 Primary map



X



Y

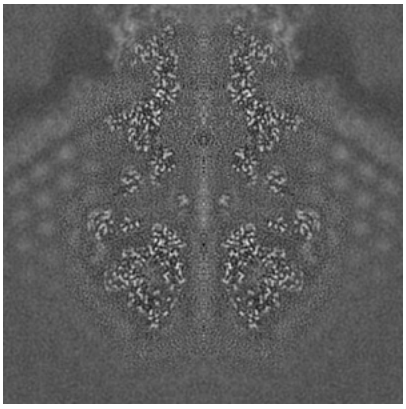


Z

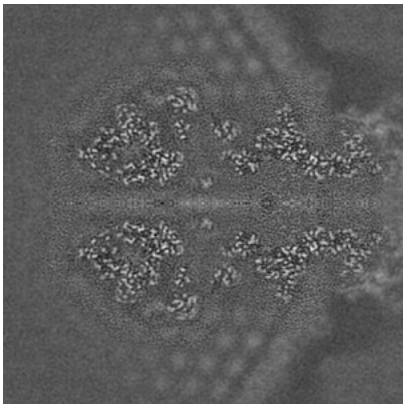
The images above show the map projected in three orthogonal directions.

6.2 Central slices

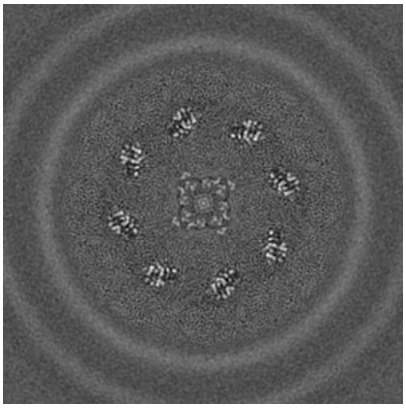
6.2.1 Primary map



X Index: 144



Y Index: 144

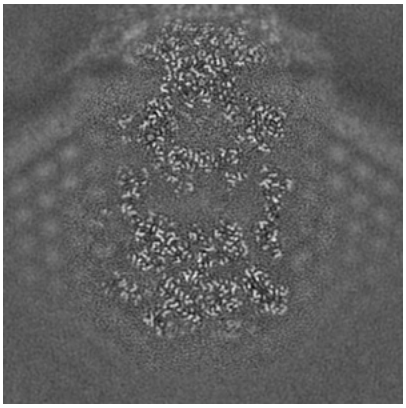


Z Index: 144

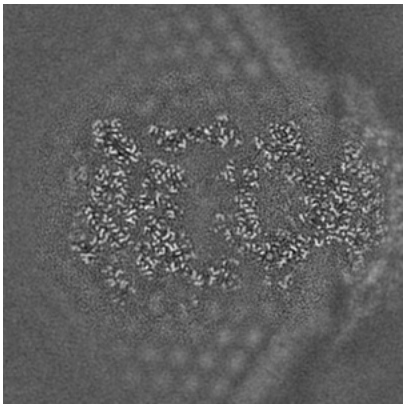
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

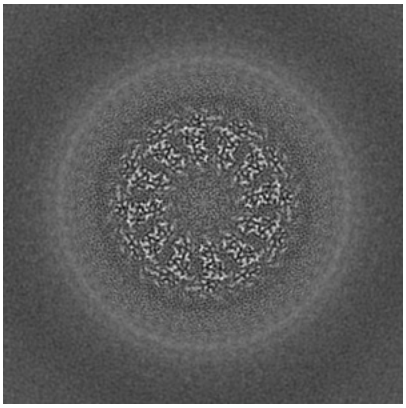
6.3.1 Primary map



X Index: 167



Y Index: 121

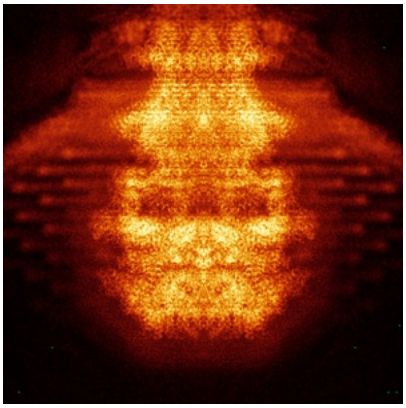


Z Index: 206

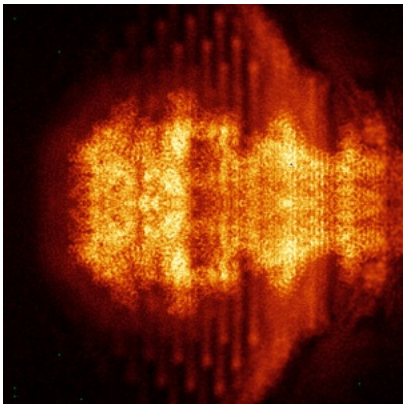
The images above show the largest variance slices of the map in three orthogonal directions.

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

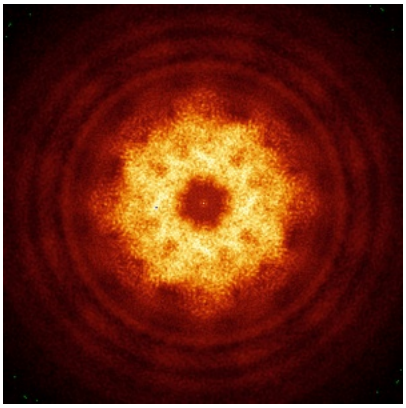
6.4.1 Primary map



X



Y

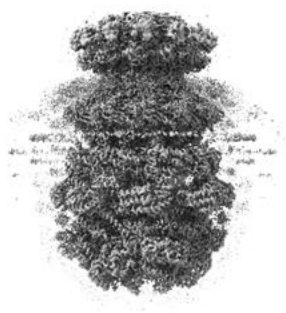


Z

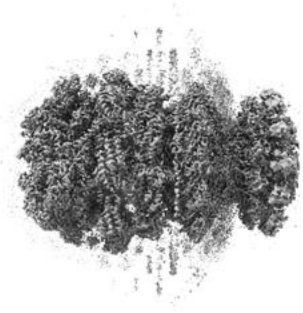
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

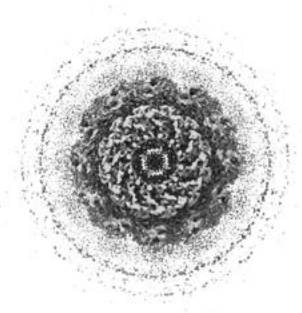
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

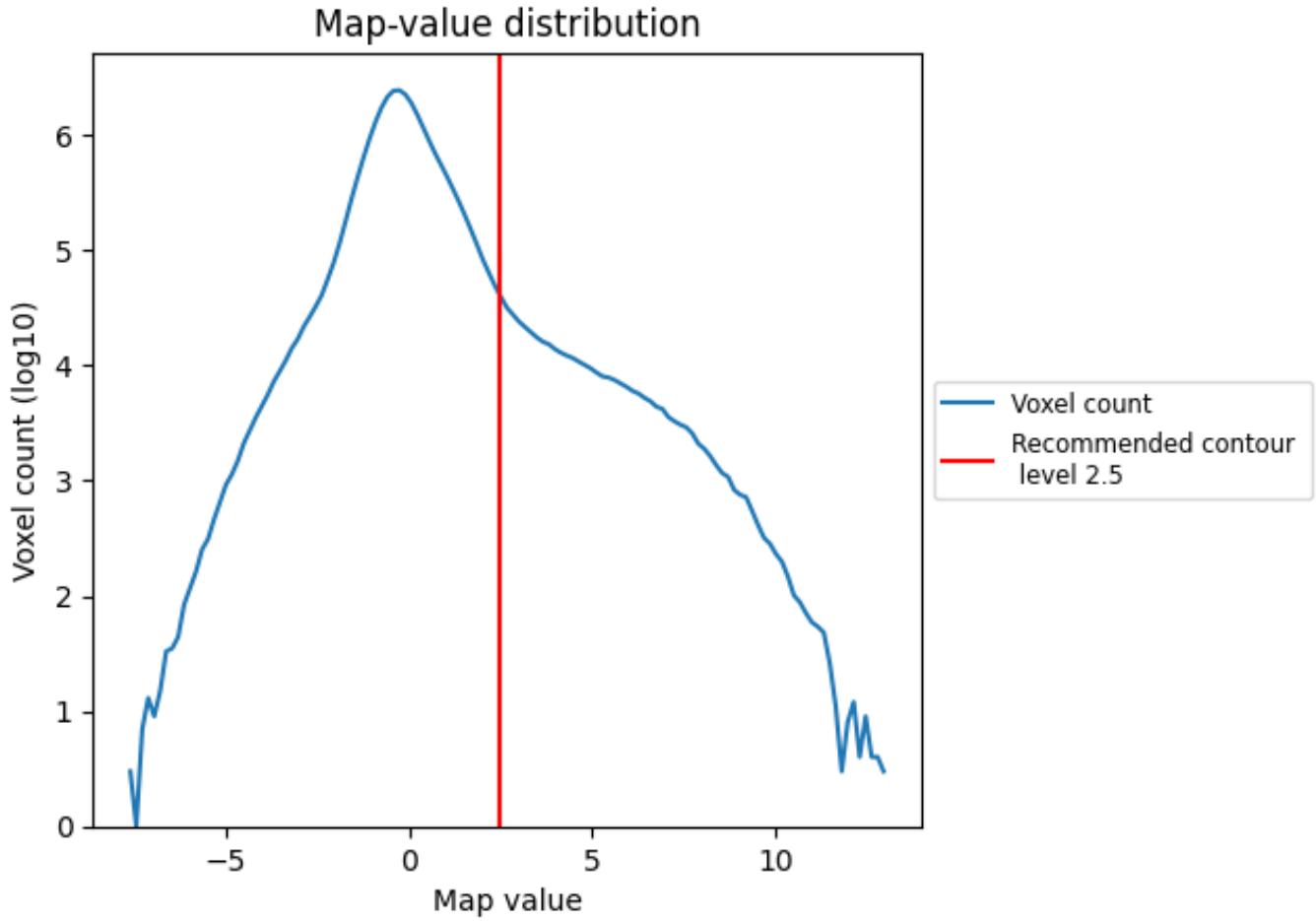
6.6 Mask visualisation (i)

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

7 Map analysis

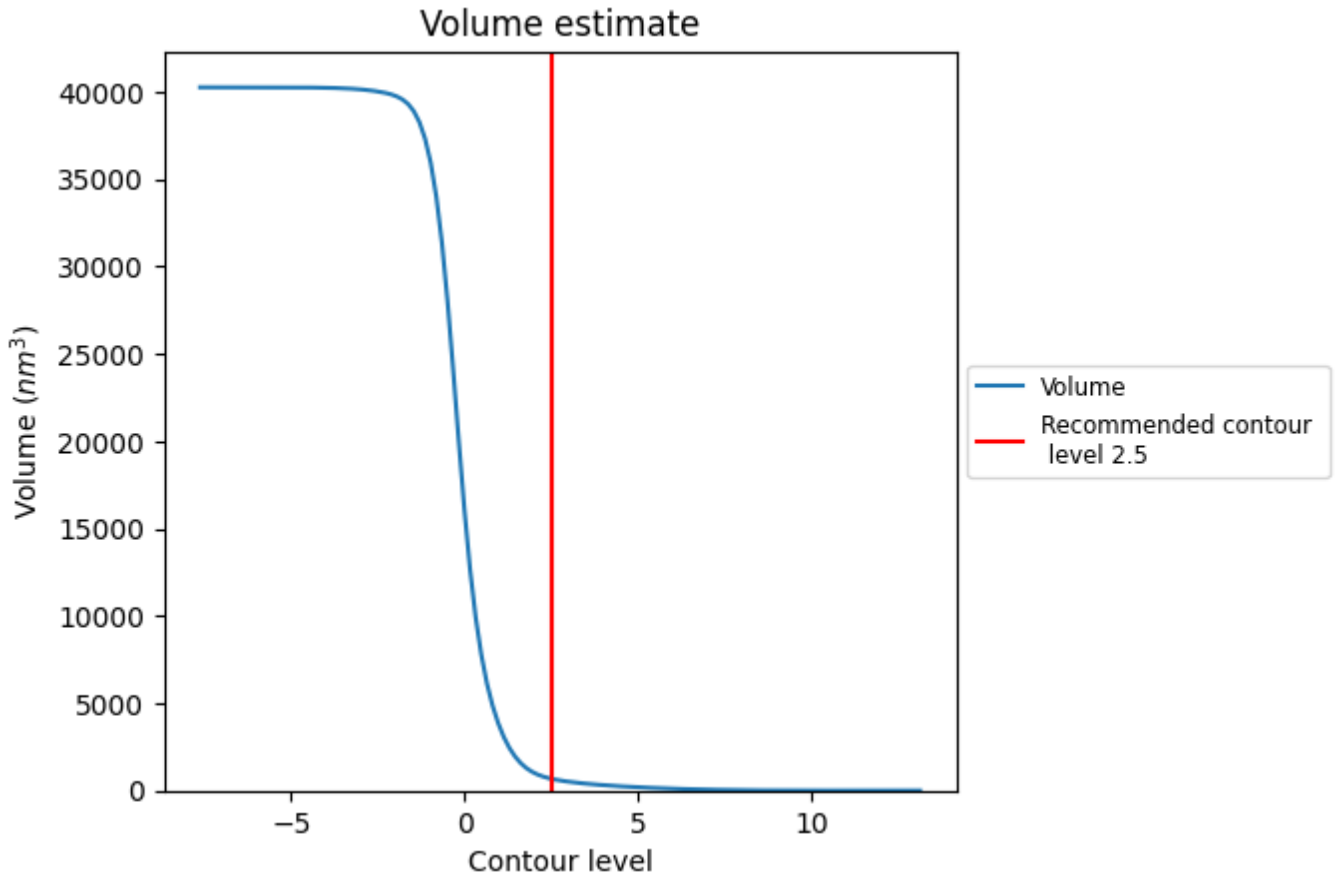
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

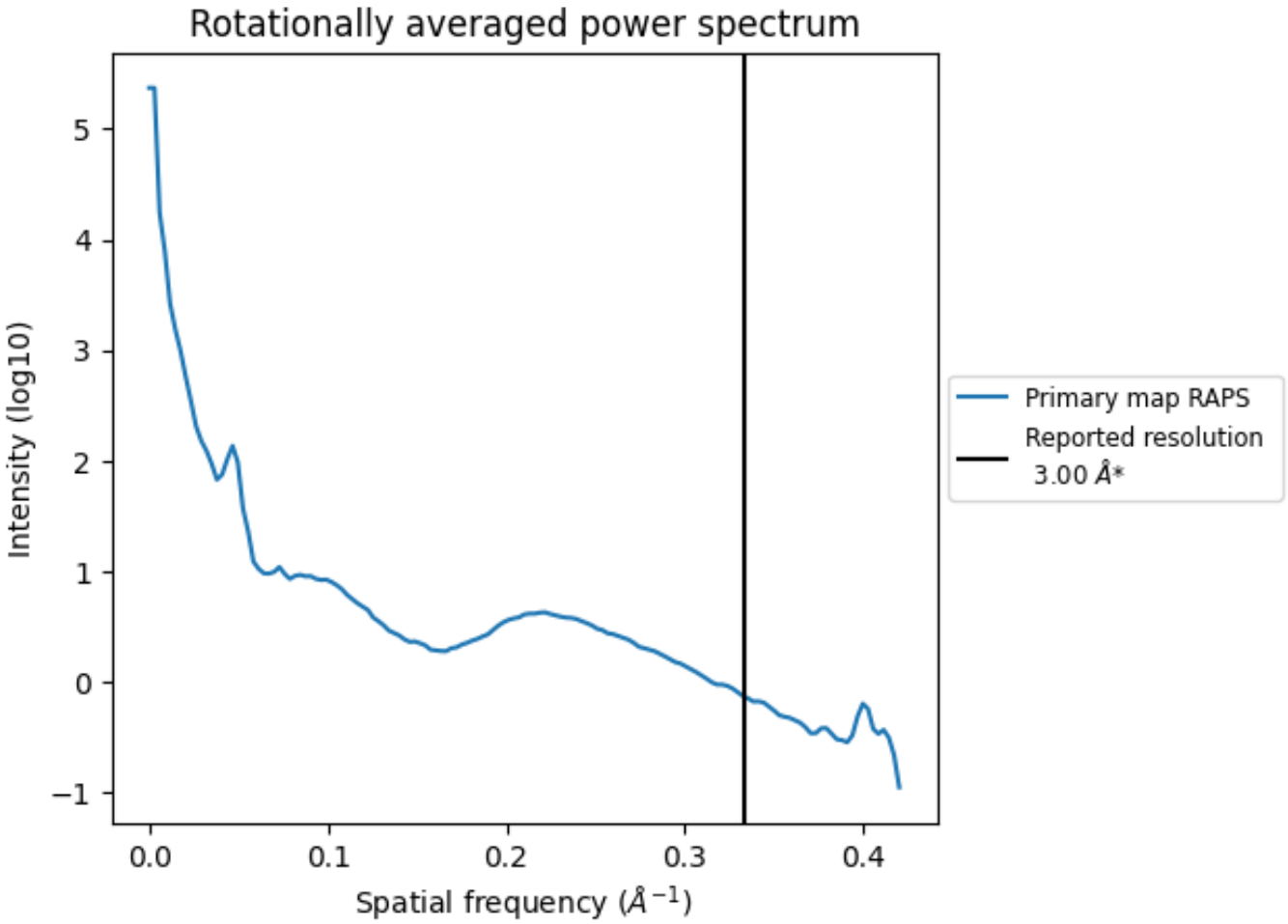
7.2 Volume estimate (i)



The volume at the recommended contour level is 679 nm^3; this corresponds to an approximate mass of 614 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 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

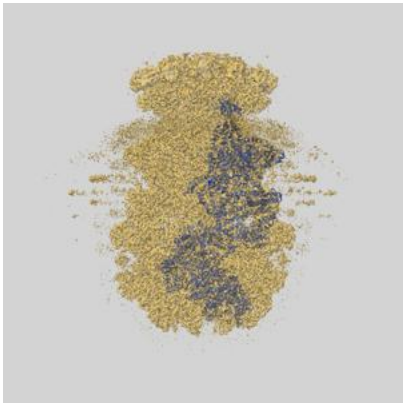
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

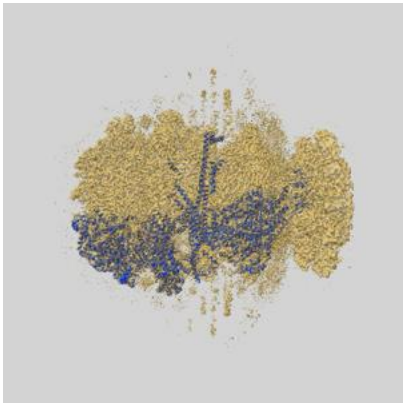
This section contains information regarding the fit between EMDB map EMD-69208 and PDB model 23SG. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

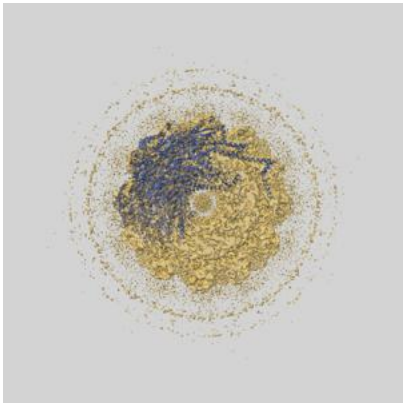
9.1.1 Map-model overlay



X

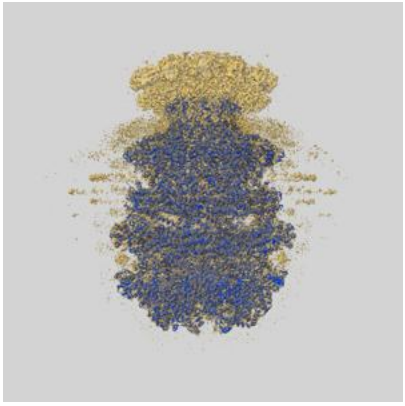


Y

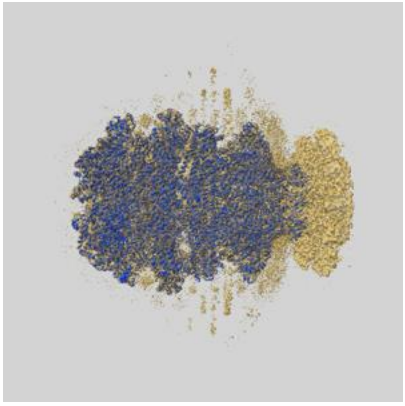


Z

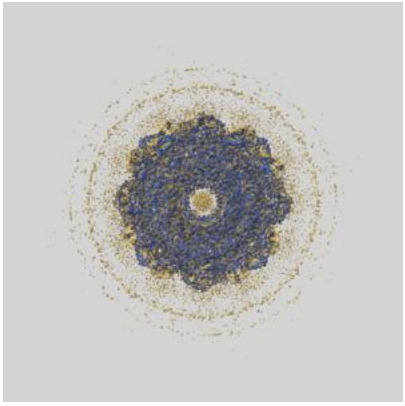
9.1.2 Map-model assembly overlay



X



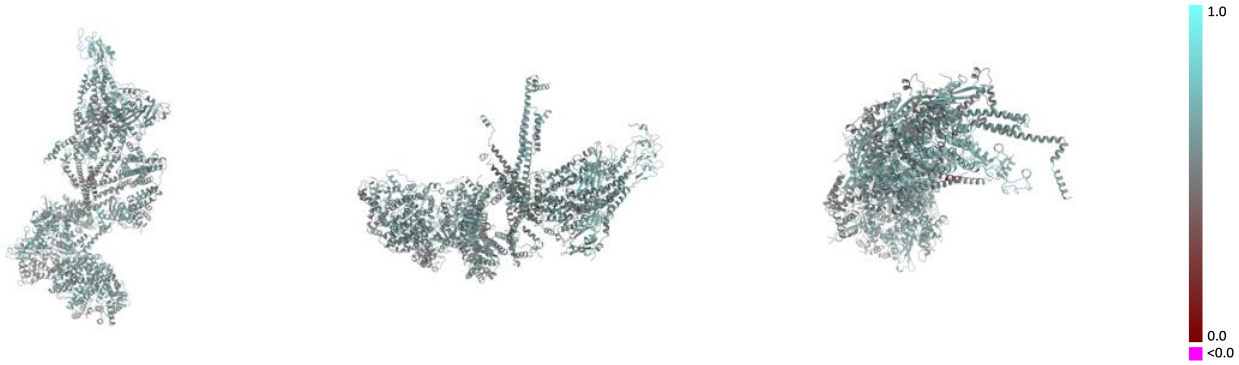
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

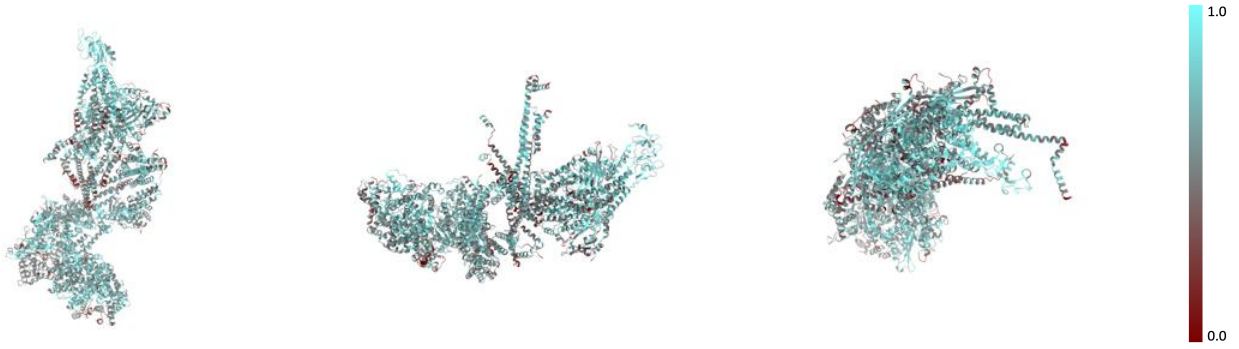
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

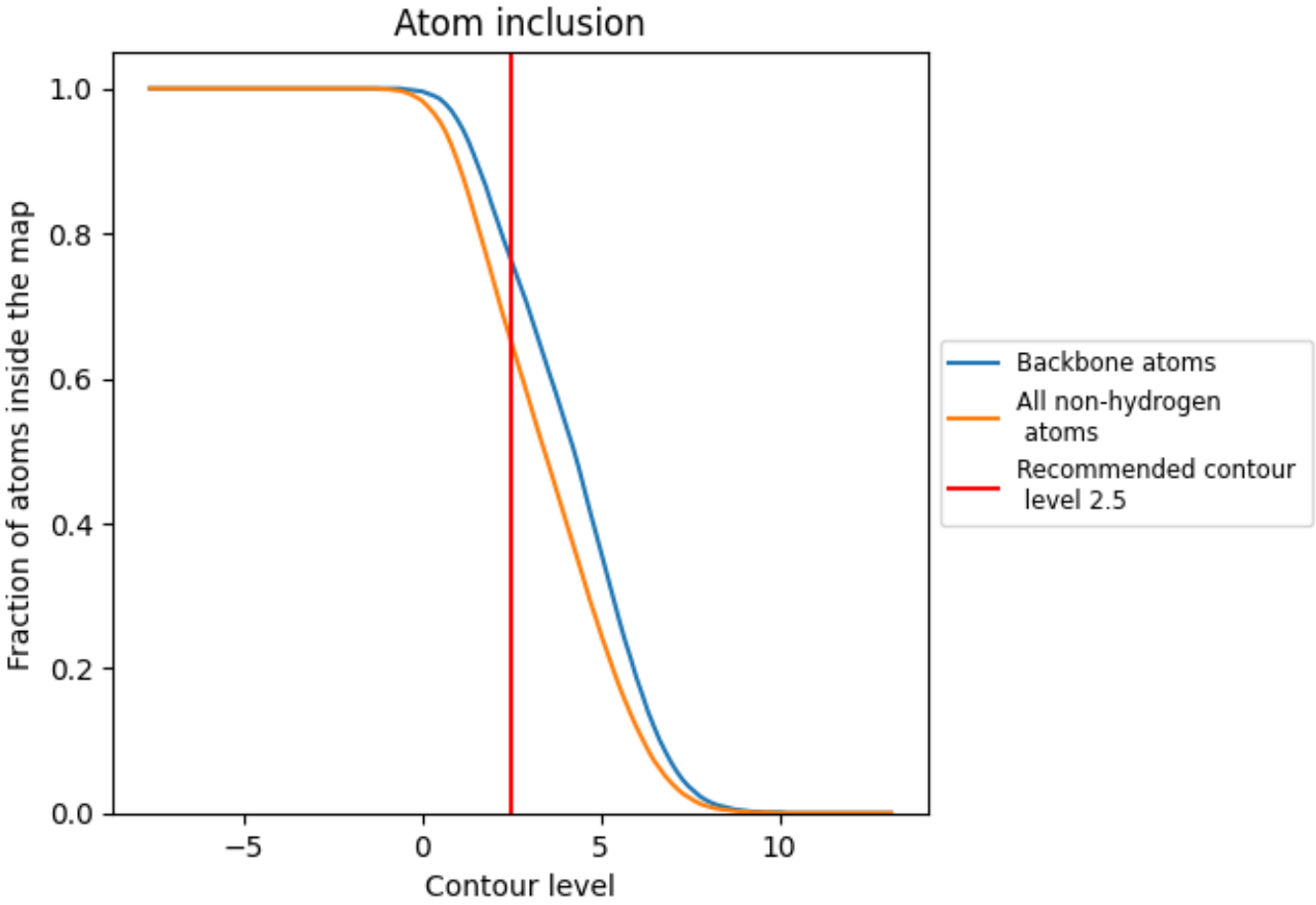
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 65% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.5710
A	0.6730	0.5820
D	0.6590	0.5780
G	0.6800	0.5760
N	0.6900	0.5810
S	0.6220	0.5610
X	0.4780	0.5200
a	0.4800	0.5170
d	0.6790	0.5820
g	0.5390	0.5730
m	0.5390	0.5500

