



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 03:50 PM EDT

PDB ID : 5VJ6
EMDB ID : EMD-8695
Title : BG505 SOSIP.664 in complex with broadly neutralizing antibodies PG9 and 8ANC195
Authors : Wang, H.; Bjorkman, P.J.
Deposited on : 2017-04-18
Resolution : 11.50 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:

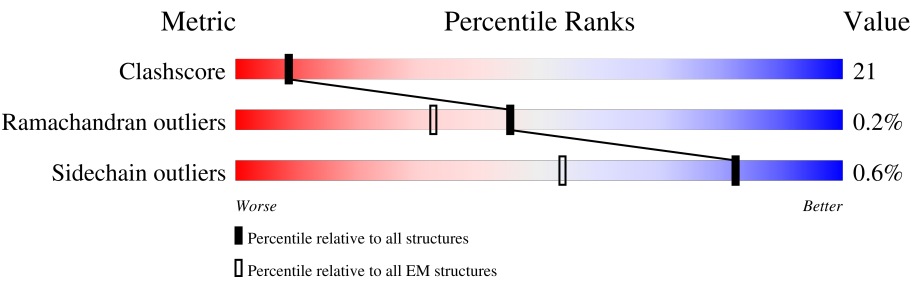
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 11.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	<div><div>18%</div><div>56%</div><div>27%</div><div>18%</div></div>
1	B	153	<div><div>22%</div><div>58%</div><div>25%</div><div>18%</div></div>
1	C	153	<div><div>14%</div><div>54%</div><div>28%</div><div>18%</div></div>
2	D	481	<div><div>20%</div><div>58%</div><div>34%</div><div>7%</div></div>
2	E	481	<div><div>24%</div><div>58%</div><div>34%</div><div>7%</div></div>
2	F	481	<div><div>20%</div><div>59%</div><div>33%</div><div>7%</div></div>
3	H	248	<div><div>35%</div><div>59%</div><div>31%</div><div>8%</div></div>
4	M	233	<div><div>19%</div><div>80%</div><div>16%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	O	233	
4	Q	233	
5	N	215	
5	P	215	
5	R	215	
6	L	216	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26459 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		
1	B	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		
1	C	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	engineered mutation	UNP Q2N0S6
A	605	CYS	THR	engineered mutation	UNP Q2N0S6
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
C	559	PRO	ILE	engineered mutation	UNP Q2N0S6
C	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
2	E	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
2	F	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	332	ASN	THR	engineered mutation	UNP Q2N0S6
D	501	CYS	ALA	engineered mutation	UNP Q2N0S6
D	509	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	510	ARG	-	expression tag	UNP Q2N0S6
D	511	ARG	-	expression tag	UNP Q2N0S6
D	512	ARG	-	expression tag	UNP Q2N0S6
D	513	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	engineered mutation	UNP Q2N0S6
F	501	CYS	ALA	engineered mutation	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called PG9 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	229	Total	C	N	O	S	0	0
			1772	1117	297	349	9		

- Molecule 4 is a protein called 8ANC195 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	224	Total	C	N	O	S	0	0
			1614	1022	269	318	5		
4	O	224	Total	C	N	O	S	0	0
			1614	1022	269	318	5		
4	Q	224	Total	C	N	O	S	0	0
			1614	1022	269	318	5		

- Molecule 5 is a protein called 8ANC195 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	214	Total	C	N	O	S	0	0
			1560	976	260	319	5		
5	P	214	Total	C	N	O	S	0	0
			1560	976	260	319	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	214	Total	C	N	O	S	0	0
			1560	976	260	319	5		

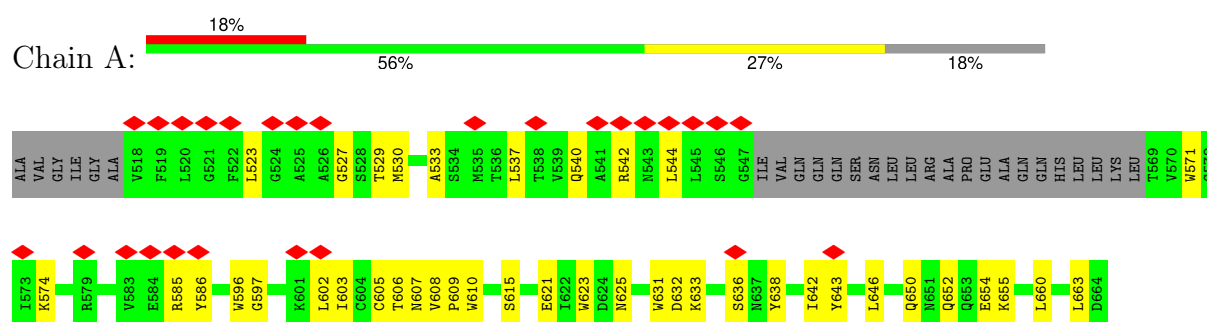
- Molecule 6 is a protein called PG9 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	211	Total	C	N	O	S	0	0
			1566	974	267	321	4		

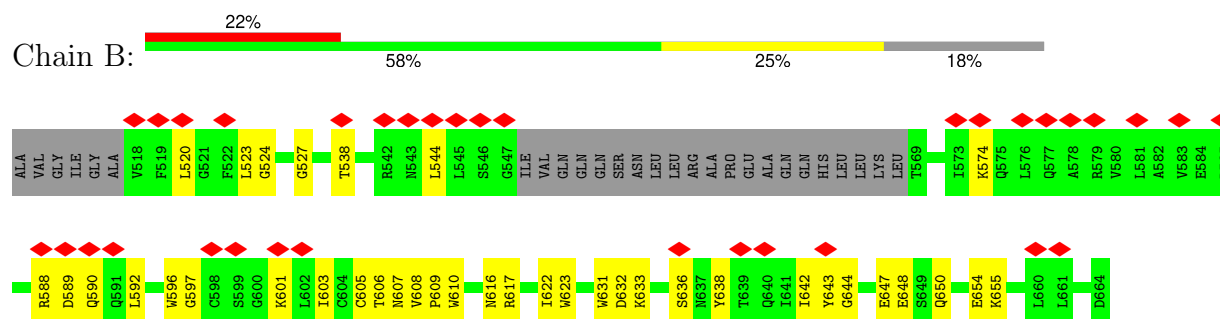
3 Residue-property plots [i](#)

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.

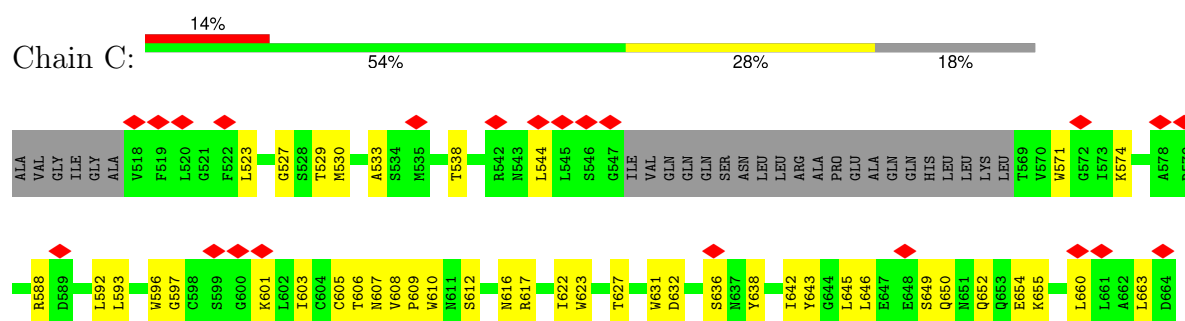
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

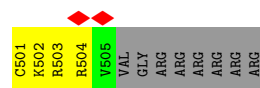


- Molecule 1: Envelope glycoprotein gp160

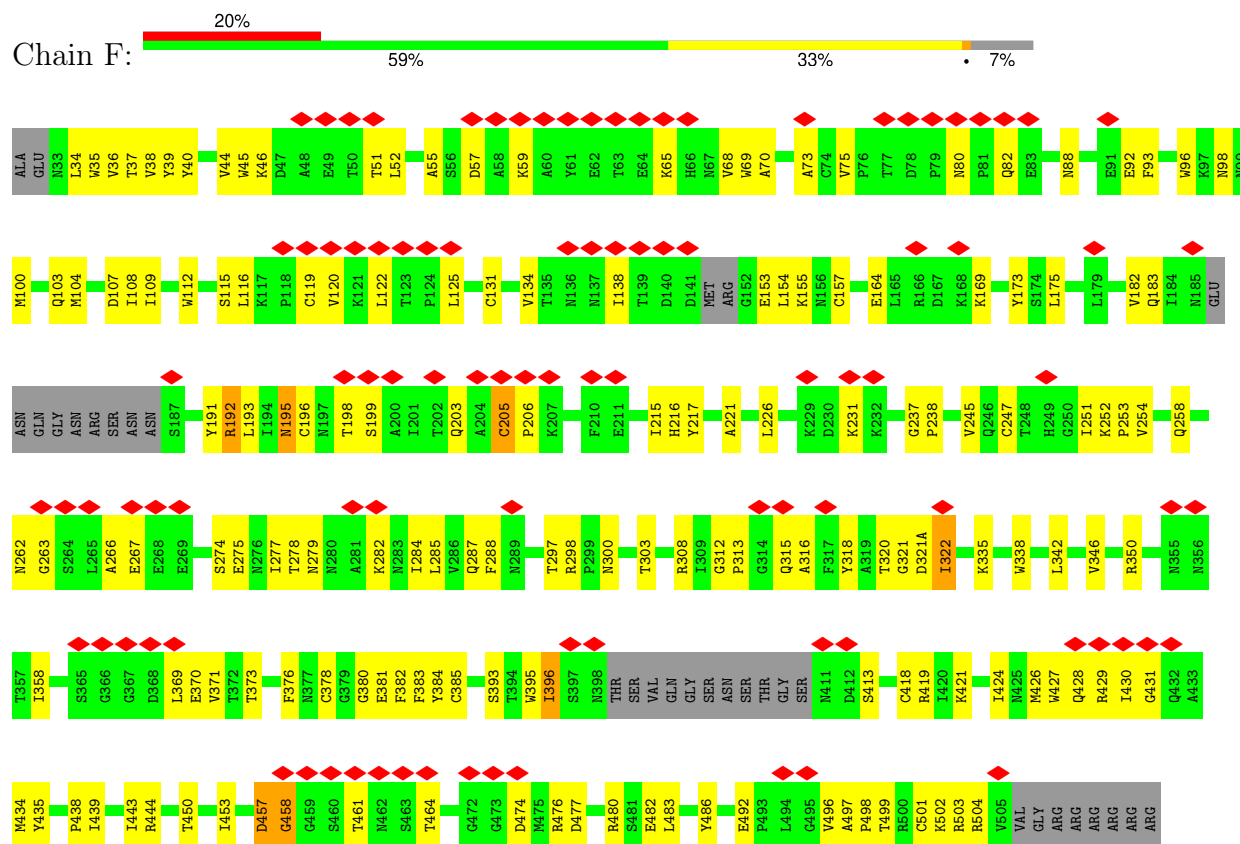


- Molecule 2: Envelope glycoprotein gp160

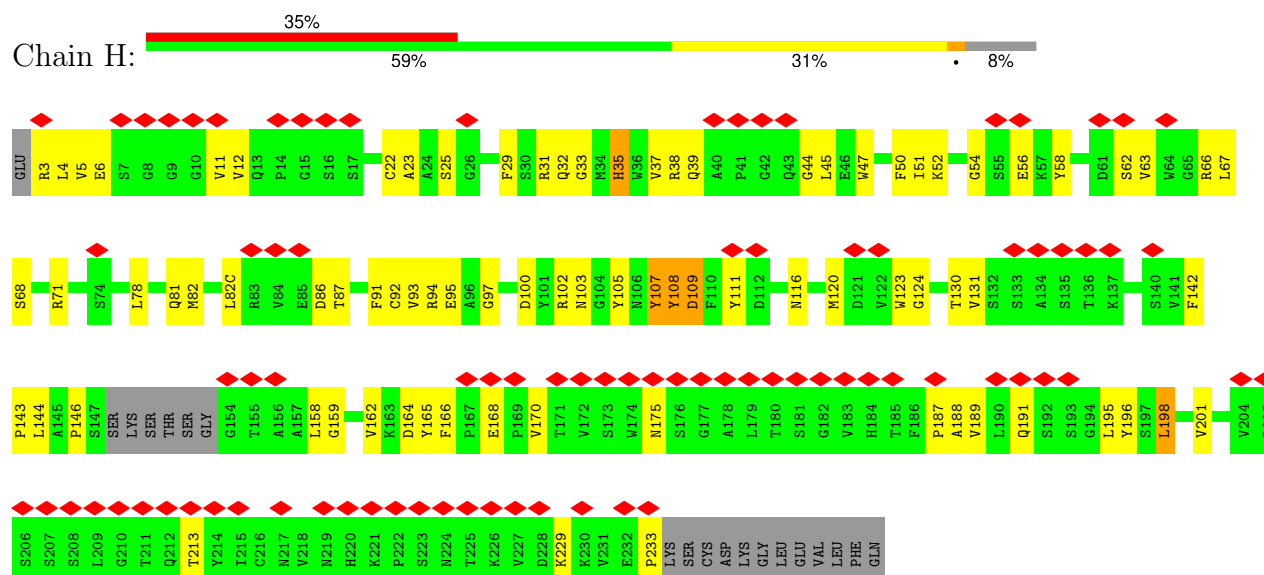




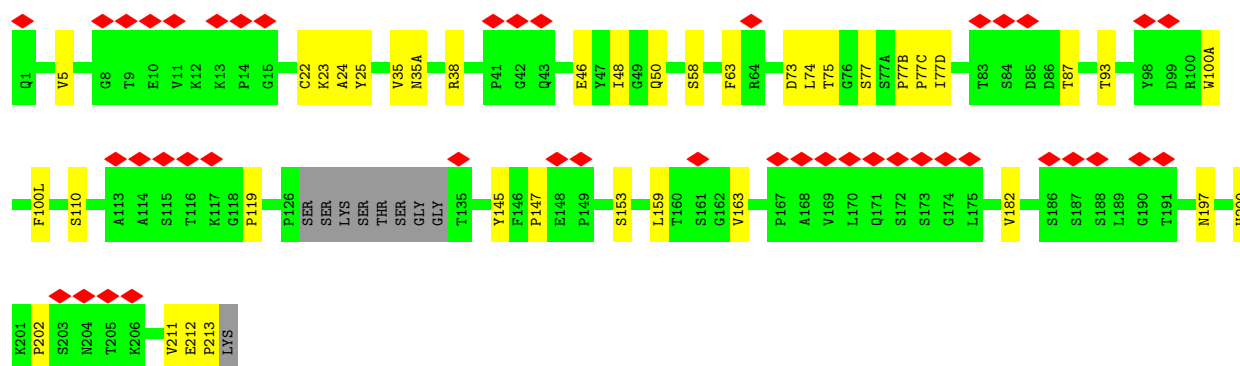
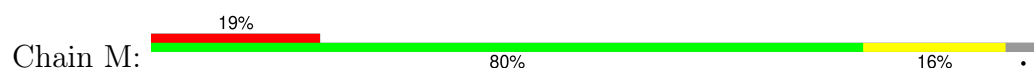
• Molecule 2: Envelope glycoprotein gp160



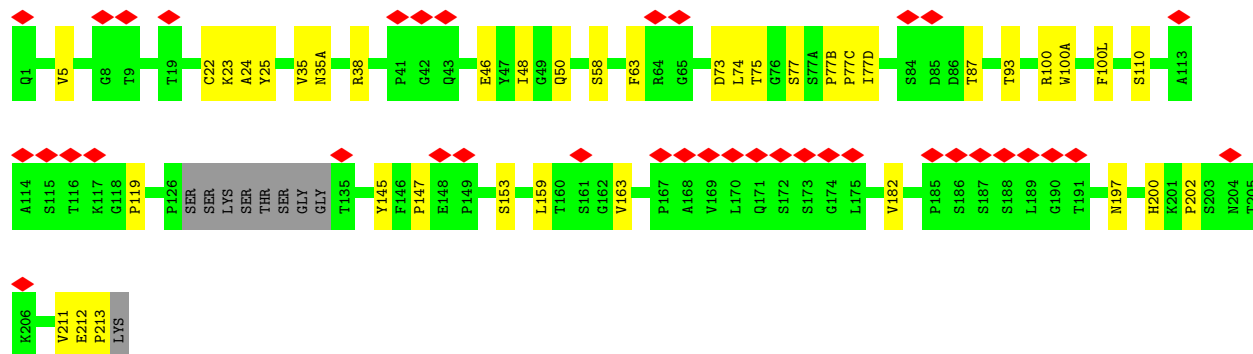
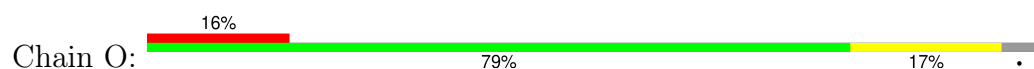
• Molecule 3: PG9 Fab heavy chain



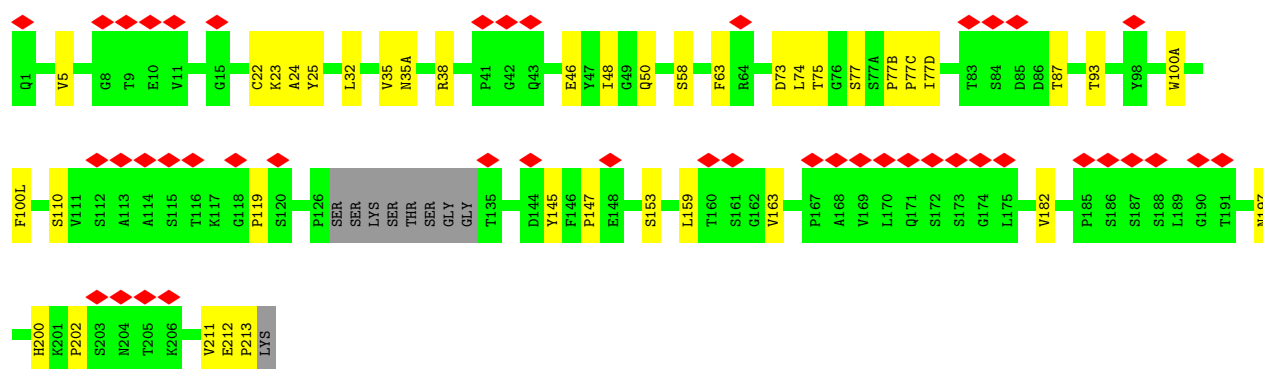
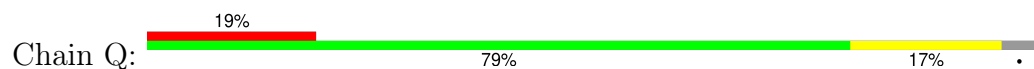
• Molecule 4: 8ANC195 Fab heavy chain



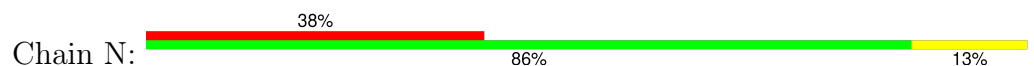
• Molecule 4: 8ANC195 Fab heavy chain

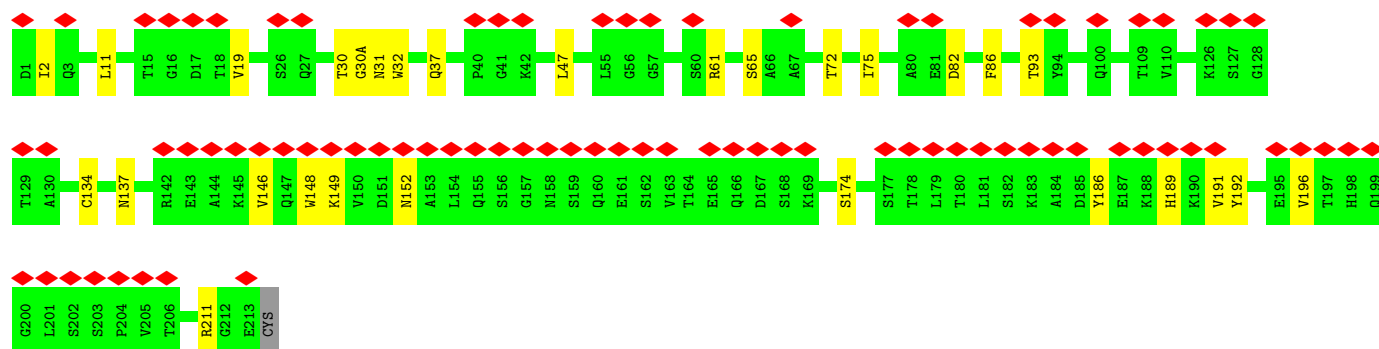


• Molecule 4: 8ANC195 Fab heavy chain

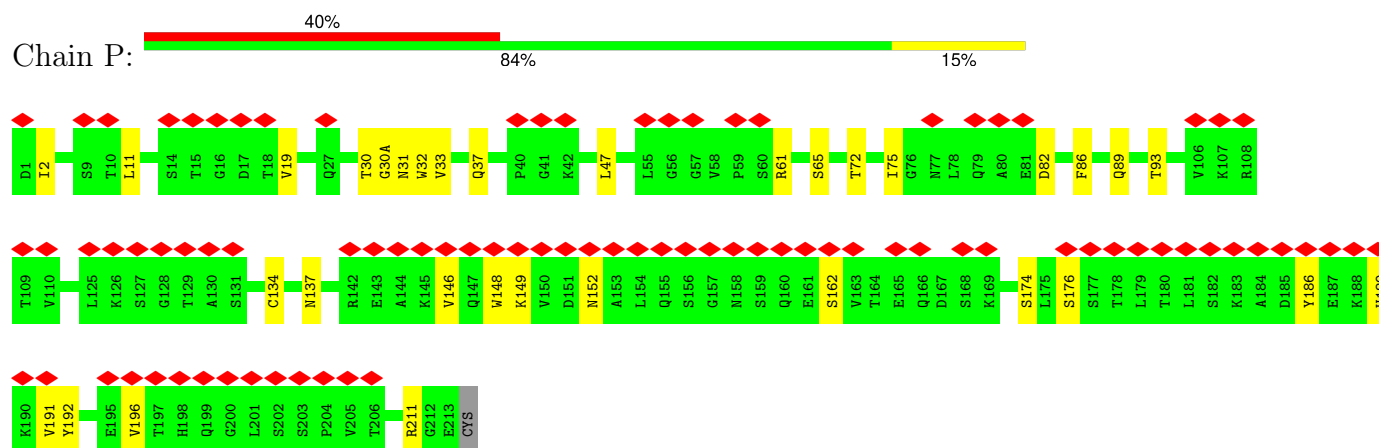


• Molecule 5: 8ANC195 Fab light chain

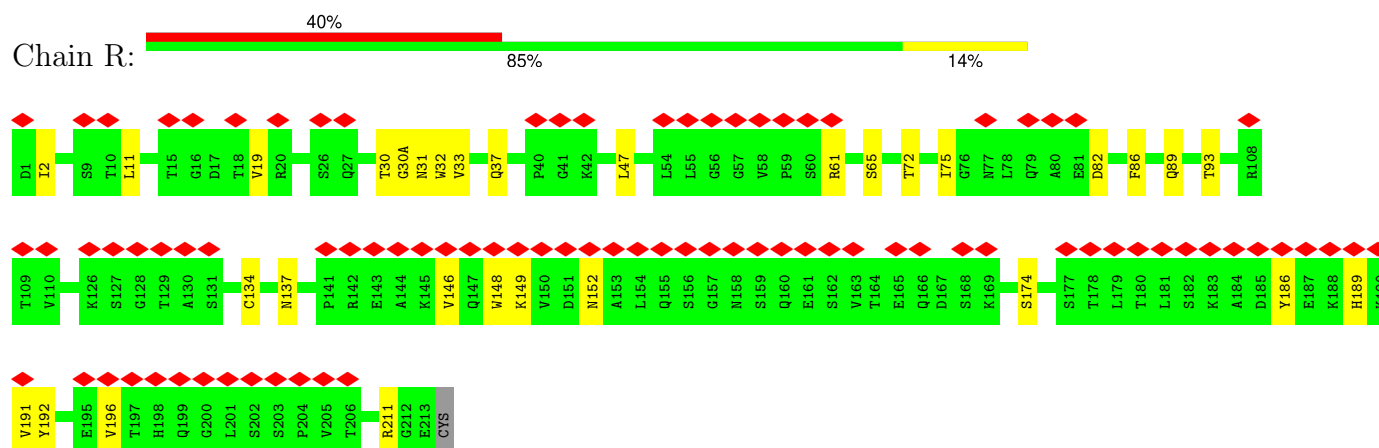




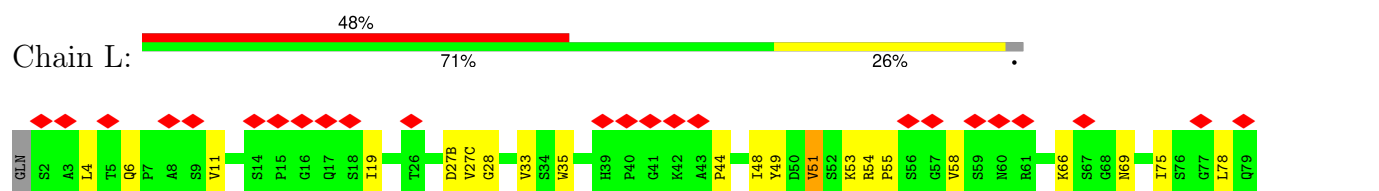
• Molecule 5: 8ANC195 Fab light chain

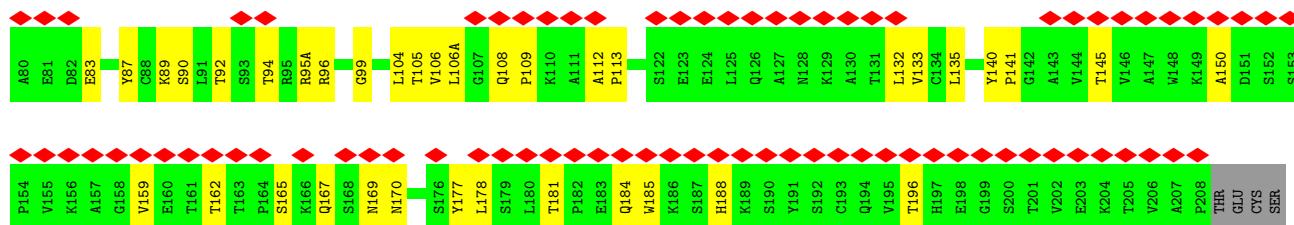


• Molecule 5: 8ANC195 Fab light chain



• Molecule 6: PG9 Fab light chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9500	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 ($e^-/\text{\AA}^2$)	30	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	0.204	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.101	Depositor
Map size (Å)	332.5, 332.5, 332.5	wwPDB
Map dimensions	190, 190, 190	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

Bond lengths and bond angles in the following residue types are not validated in this section: TYS

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	0.27	0/1019	0.55	0/1382
1	B	0.27	0/1019	0.58	0/1382
1	C	0.26	0/1019	0.56	0/1382
2	D	0.28	0/3605	0.53	2/4895 (0.0%)
2	E	0.28	0/3605	0.53	2/4895 (0.0%)
2	F	0.28	0/3605	0.53	2/4895 (0.0%)
3	H	0.32	0/1786	0.62	1/2429 (0.0%)
4	M	0.31	1/1656 (0.1%)	0.50	1/2280 (0.0%)
4	O	0.31	1/1656 (0.1%)	0.50	1/2280 (0.0%)
4	Q	0.31	1/1656 (0.1%)	0.50	1/2280 (0.0%)
5	N	0.26	0/1594	0.46	0/2181
5	P	0.26	0/1594	0.46	0/2181
5	R	0.26	0/1594	0.46	0/2181
6	L	0.29	0/1601	0.51	0/2180
All	All	0.28	3/27009 (0.0%)	0.52	10/36823 (0.0%)

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
3	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	213	PRO	N-CD	5.22	1.55	1.47
4	Q	213	PRO	N-CD	5.22	1.55	1.47
4	O	213	PRO	N-CD	5.18	1.55	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	458	GLY	O-C-N	-8.00	109.60	123.20
2	E	458	GLY	O-C-N	-7.99	109.62	123.20
2	F	458	GLY	O-C-N	-7.98	109.64	123.20
3	H	198	LEU	CA-CB-CG	6.12	129.38	115.30
2	E	458	GLY	CA-C-N	5.83	127.85	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	35	HIS	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	1001	0	978	177	0
1	B	1001	0	977	151	0
1	C	1001	0	977	144	0
2	D	3532	0	3480	261	0
2	E	3532	0	3479	261	0
2	F	3532	0	3479	232	0
3	H	1772	0	1670	98	0
4	M	1614	0	1511	46	0
4	O	1614	0	1511	49	0
4	Q	1614	0	1511	47	0
5	N	1560	0	1438	21	0
5	P	1560	0	1438	22	0
5	R	1560	0	1438	27	0
6	L	1566	0	1533	69	0
All	All	26459	0	25420	1072	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 1072 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)
1:A:636:SER:CB	4:O:100(A):TRP:HZ3	1.15	1.58
1:A:605:CYS:SG	2:D:501:CYS:SG	1.47	1.44
3:H:95:GLU:HG3	6:L:89:LYS:NZ	1.30	1.44
1:A:636:SER:CB	4:O:100(A):TRP:CZ3	1.99	1.43
3:H:95:GLU:CG	6:L:89:LYS:NZ	1.79	1.43

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/153 (80%)	112 (92%)	10 (8%)	0	100	100
1	B	122/153 (80%)	110 (90%)	12 (10%)	0	100	100
1	C	122/153 (80%)	114 (93%)	8 (7%)	0	100	100
2	D	441/481 (92%)	406 (92%)	33 (8%)	2 (0%)	25	64
2	E	441/481 (92%)	408 (92%)	31 (7%)	2 (0%)	25	64
2	F	441/481 (92%)	407 (92%)	32 (7%)	2 (0%)	25	64
3	H	223/248 (90%)	201 (90%)	21 (9%)	1 (0%)	30	68
4	M	220/233 (94%)	210 (96%)	10 (4%)	0	100	100
4	O	220/233 (94%)	210 (96%)	10 (4%)	0	100	100
4	Q	220/233 (94%)	210 (96%)	10 (4%)	0	100	100
5	N	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
5	P	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
5	R	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
6	L	209/216 (97%)	204 (98%)	4 (2%)	1 (0%)	25	64
All	All	3417/3710 (92%)	3219 (94%)	190 (6%)	8 (0%)	45	78

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	51	VAL
2	D	138	ILE
2	E	138	ILE
2	F	138	ILE
2	D	457	ASP

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	108/129 (84%)	108 (100%)	0	100	100
1	B	108/129 (84%)	108 (100%)	0	100	100
1	C	108/129 (84%)	108 (100%)	0	100	100
2	D	401/428 (94%)	395 (98%)	6 (2%)	60	75
2	E	401/428 (94%)	395 (98%)	6 (2%)	60	75
2	F	401/428 (94%)	395 (98%)	6 (2%)	60	75
3	H	191/208 (92%)	191 (100%)	0	100	100
4	M	175/199 (88%)	175 (100%)	0	100	100
4	O	175/199 (88%)	175 (100%)	0	100	100
4	Q	175/199 (88%)	175 (100%)	0	100	100
5	N	163/182 (90%)	163 (100%)	0	100	100
5	P	163/182 (90%)	163 (100%)	0	100	100
5	R	163/182 (90%)	163 (100%)	0	100	100
6	L	178/183 (97%)	178 (100%)	0	100	100
All	All	2910/3205 (91%)	2892 (99%)	18 (1%)	82	88

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	195	ASN
2	F	396	ILE
2	F	322	ILE

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Mol	Chain	Res	Type
2	E	195	ASN
2	F	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
5	N	31	ASN
5	R	31	ASN
1	C	607	ASN
1	C	650	GLN
1	C	652	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TYS	H	108	3	15,16,17	1.63	3 (20%)	15,22,24	0.75	0
3	TYS	H	107	3	15,16,17	1.65	3 (20%)	15,22,24	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	H	108	3	-	5/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	H	107	3	-	0/10/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	107	TYS	O1-S	4.29	1.64	1.45
3	H	108	TYS	O1-S	4.29	1.63	1.45
3	H	107	TYS	OH-CZ	-3.38	1.37	1.42
3	H	108	TYS	OH-CZ	-3.18	1.37	1.42
3	H	107	TYS	OH-S	-2.45	1.53	1.58

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	108	TYS	N-CA-CB-CG
3	H	108	TYS	CZ-OH-S-O1
3	H	108	TYS	CZ-OH-S-O2
3	H	108	TYS	C-CA-CB-CG
3	H	108	TYS	CZ-OH-S-O3

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	108	TYS	5	0
3	H	107	TYS	2	0

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.

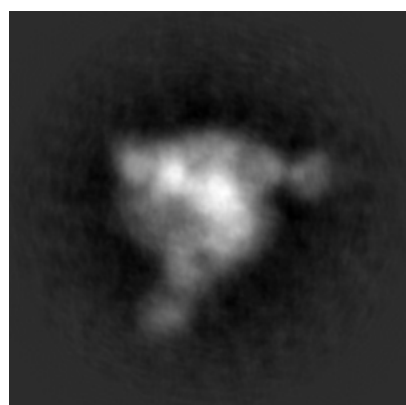
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8695. These allow visual inspection of the internal detail of the map and identification of artifacts.

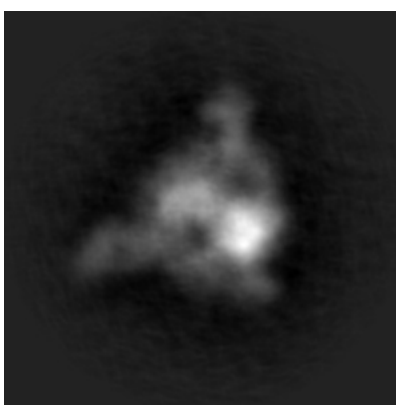
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

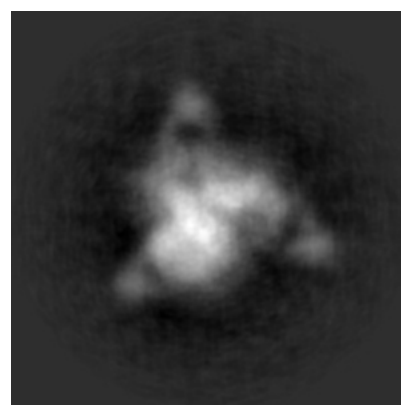
6.1.1 Primary map



X



Y

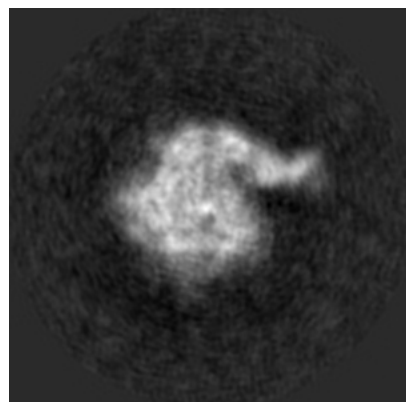


Z

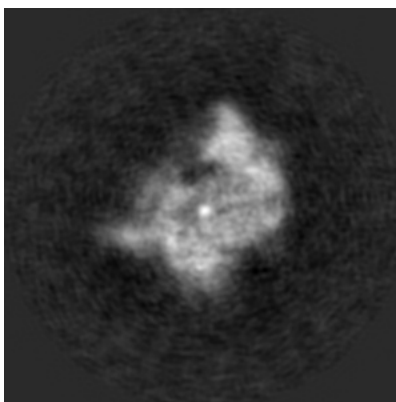
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

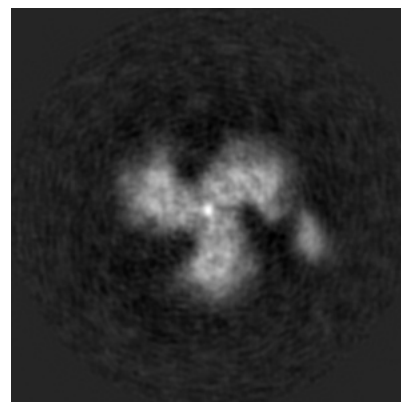
6.2.1 Primary map



X Index: 95



Y Index: 95

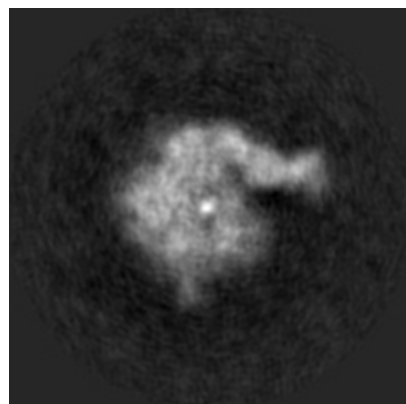


Z Index: 95

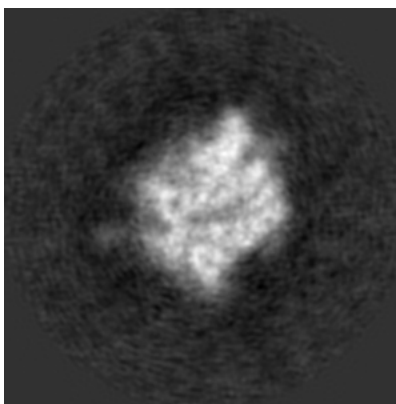
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

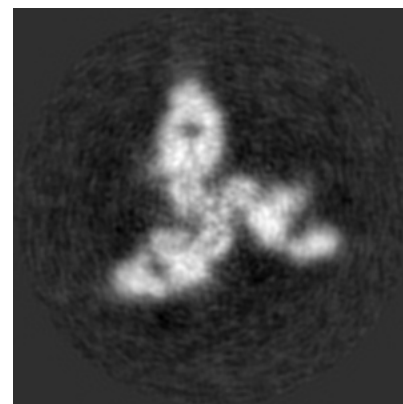
6.3.1 Primary map



X Index: 93



Y Index: 100

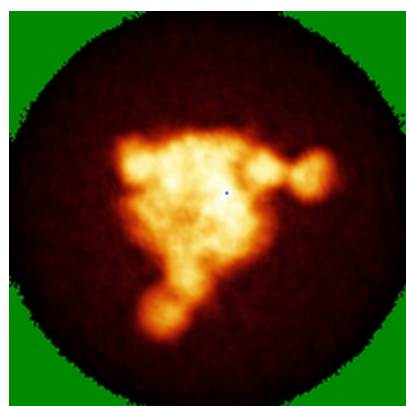


Z Index: 113

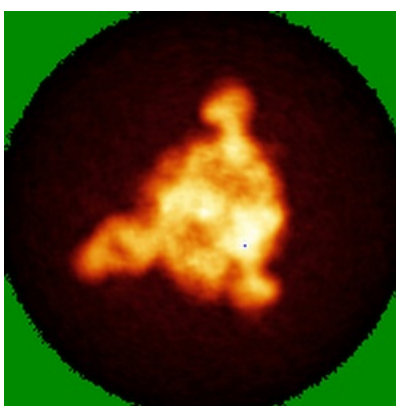
The images above show the largest variance slices of the map in three orthogonal directions.

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

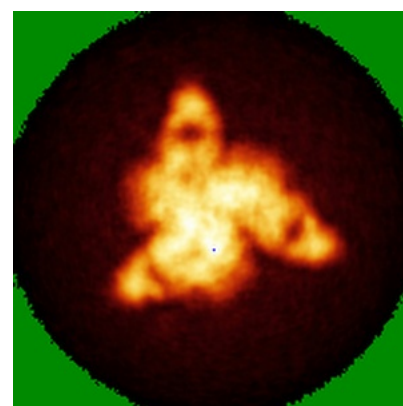
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.101. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

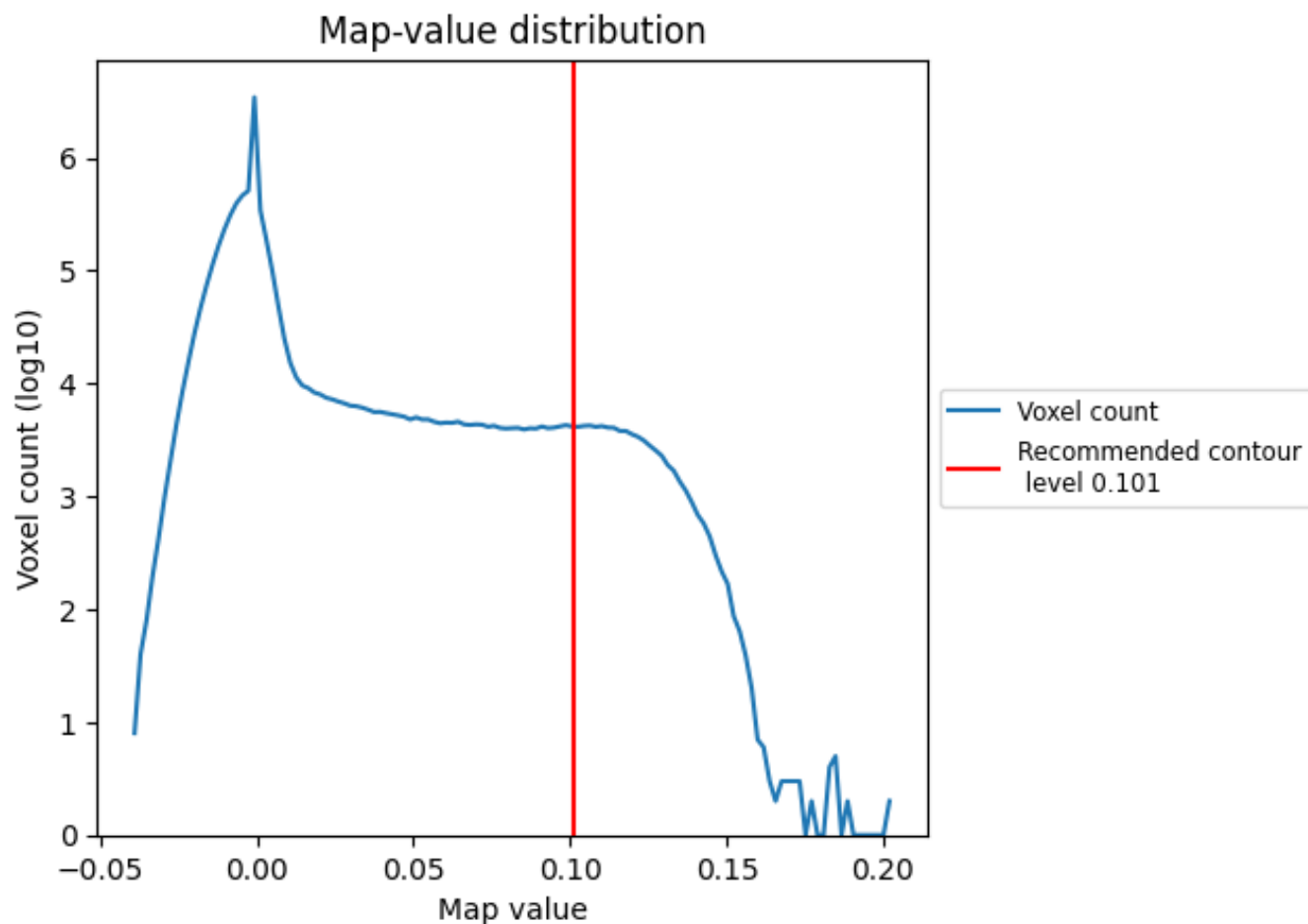
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

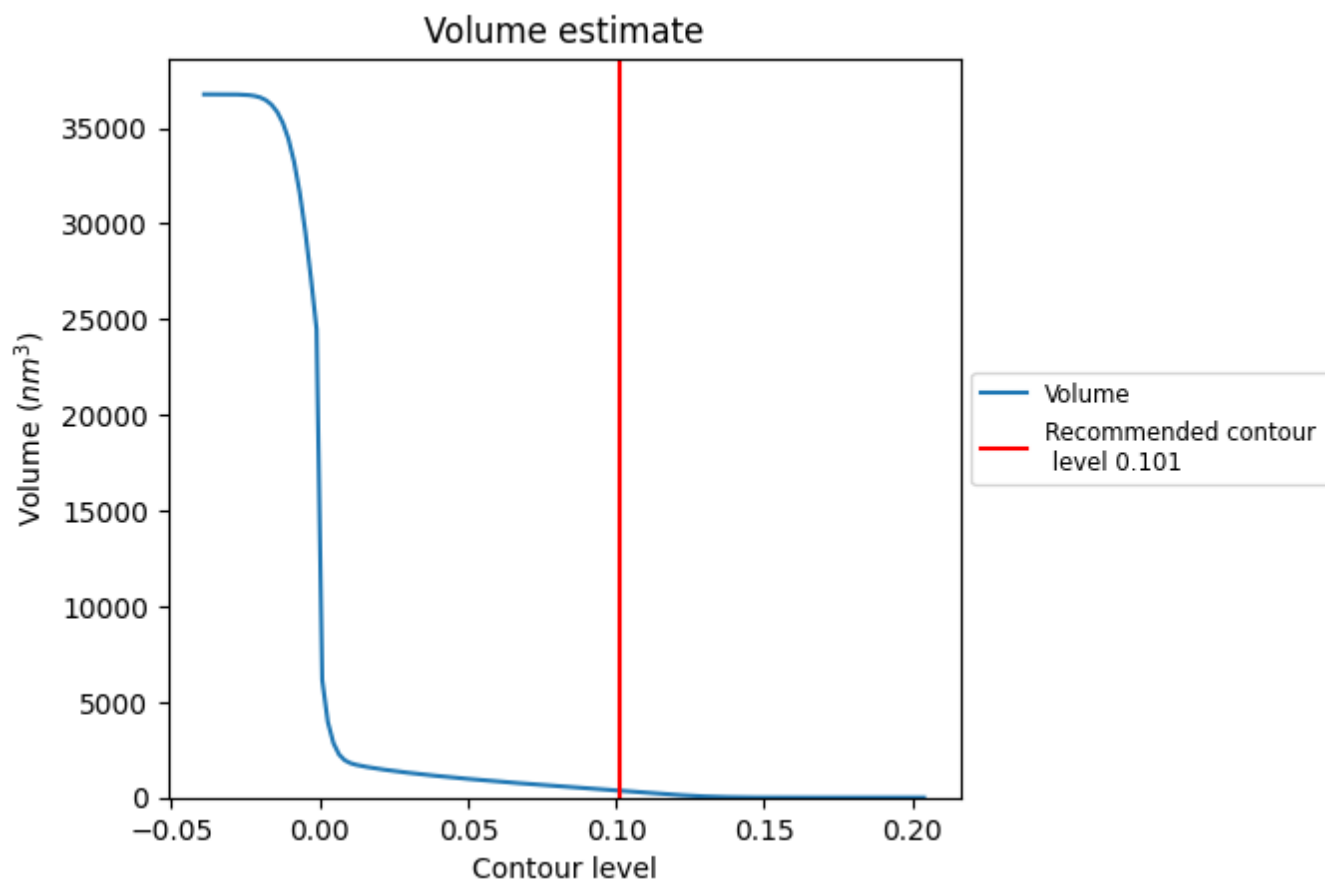
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

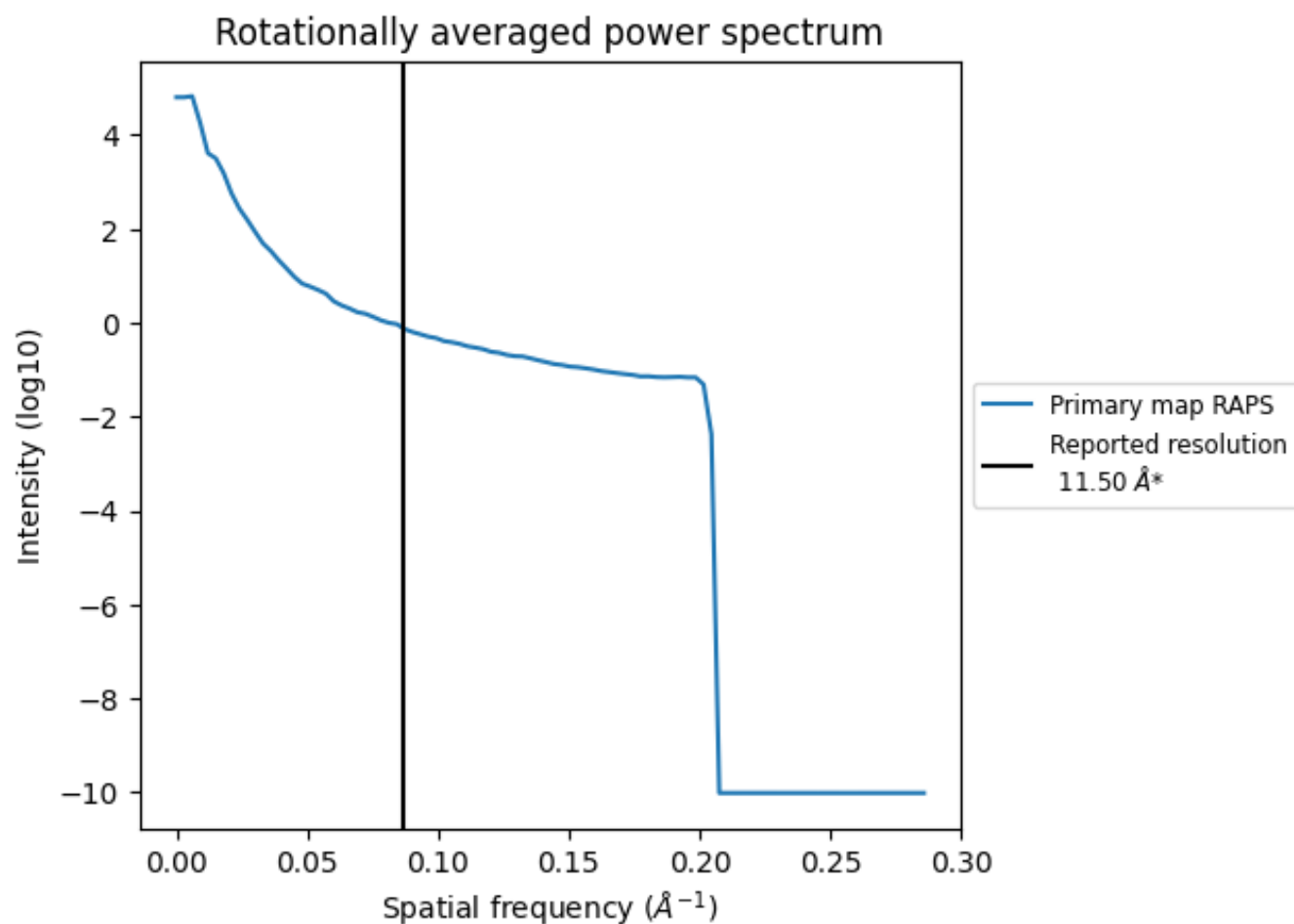
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm³; this corresponds to an approximate mass of 327 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 ⓘ

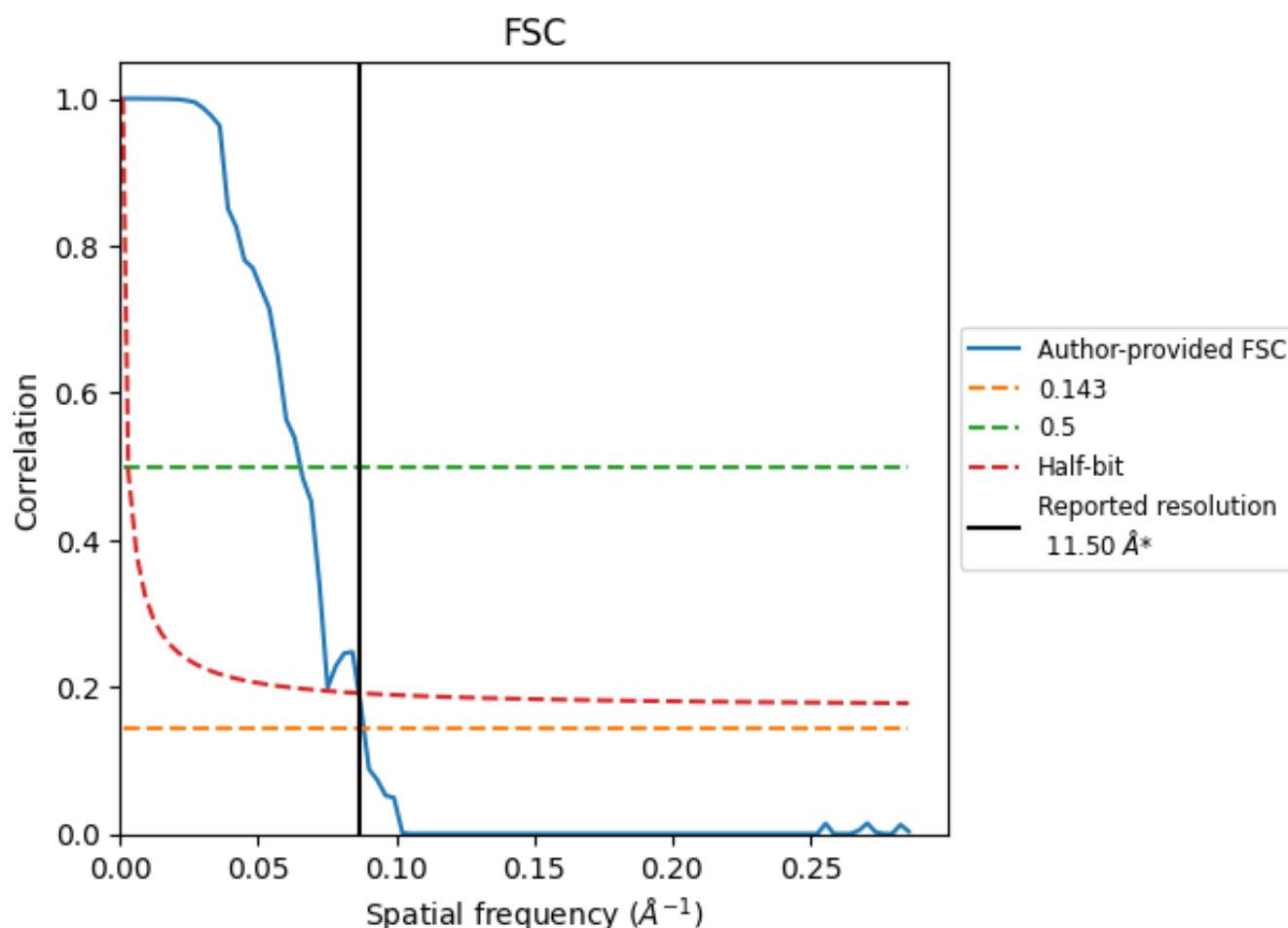


*Reported resolution corresponds to spatial frequency of 0.087 \AA^{-1}

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 0.087 Å⁻¹

8.2 Resolution estimates [i](#)

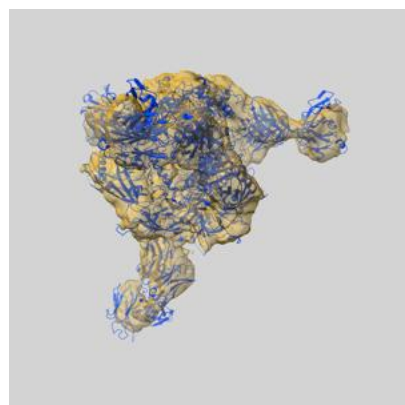
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.50	-	-
Author-provided FSC curve	11.33	15.31	11.56
Unmasked-calculated*	-	-	-

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

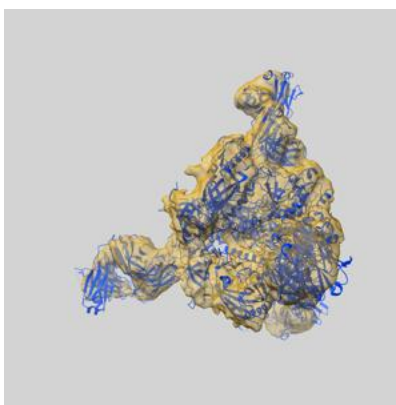
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8695 and PDB model 5VJ6. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

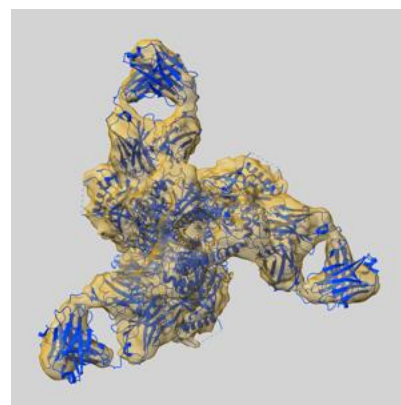
9.1 Map-model overlay [i](#)



X



Y



Z

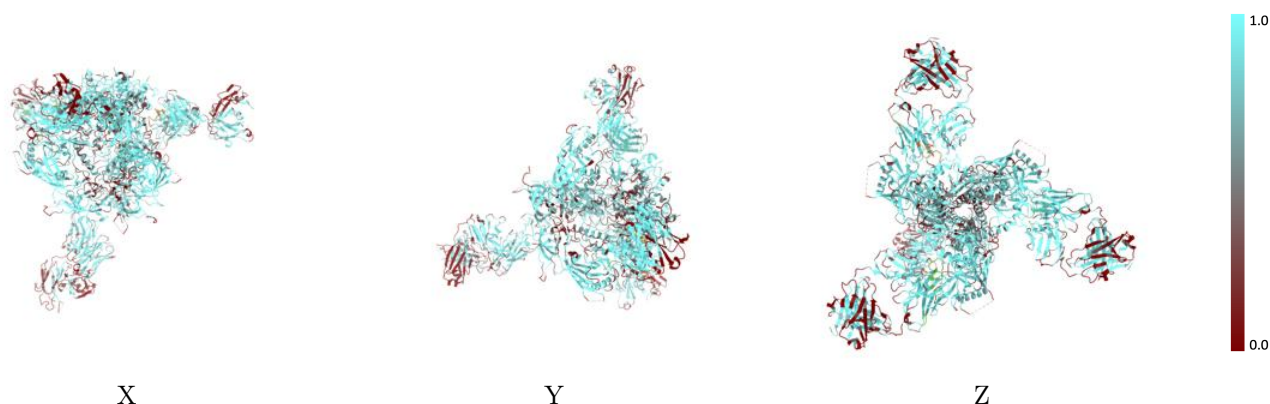
The images above show the 3D surface view of the map at the recommended contour level 0.101 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



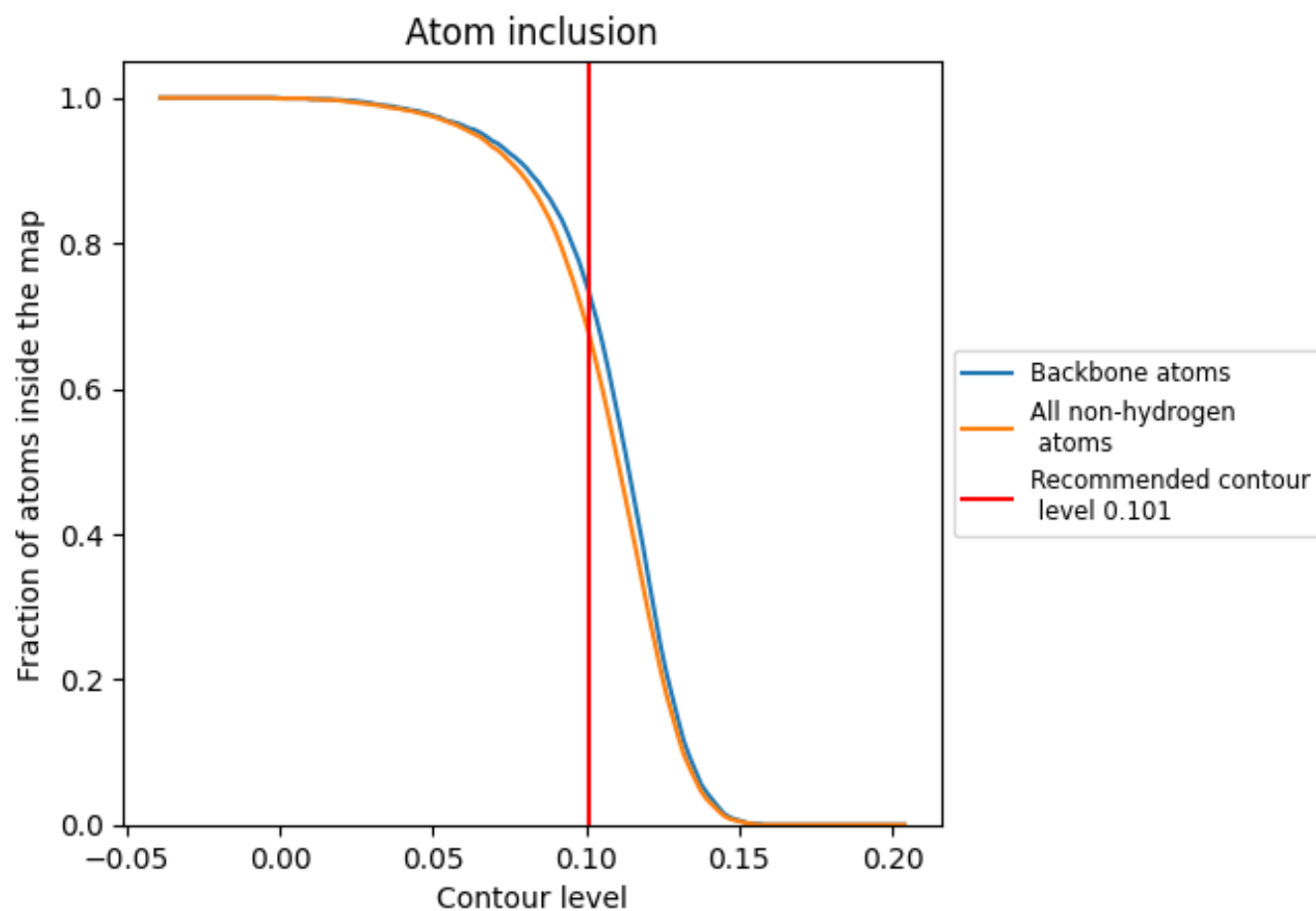
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.101).































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6740	 0.0970
A	 0.6960	 0.1110
B	 0.6640	 0.0870
C	 0.7400	 0.1100
D	 0.7240	 0.1030
E	 0.6910	 0.1020
F	 0.7110	 0.0980
H	 0.6070	 0.1040
L	 0.4640	 0.0850
M	 0.7720	 0.0990
N	 0.5910	 0.0850
O	 0.7730	 0.0880
P	 0.5720	 0.0860
Q	 0.7600	 0.1020
R	 0.5630	 0.0820

