wwPDB EM Validation Summary Report

Sep 20, 2026 – 12:23 PM EDT

PDB ID	:	11LQ / pdb_000011lq
EMDB ID	:	EMD-75813
Title	:	Human monoclonal antibodies 4C12 and 4H3 in complex with rabies virus glycoprotein
Authors	:	Callaway, H.M.; Zyla, D.; Hastie, K.; Harkins, S.; Kothalawalage, S.; Samarasinghe, S.; Flynn, A.; Hariharan, C.; Yin, J.; Corti, D.; Bouhry, H.; Dessain, S.; Saphire, E.O.
Deposited on	:	2026-03-03
Resolution	:	3.24 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:

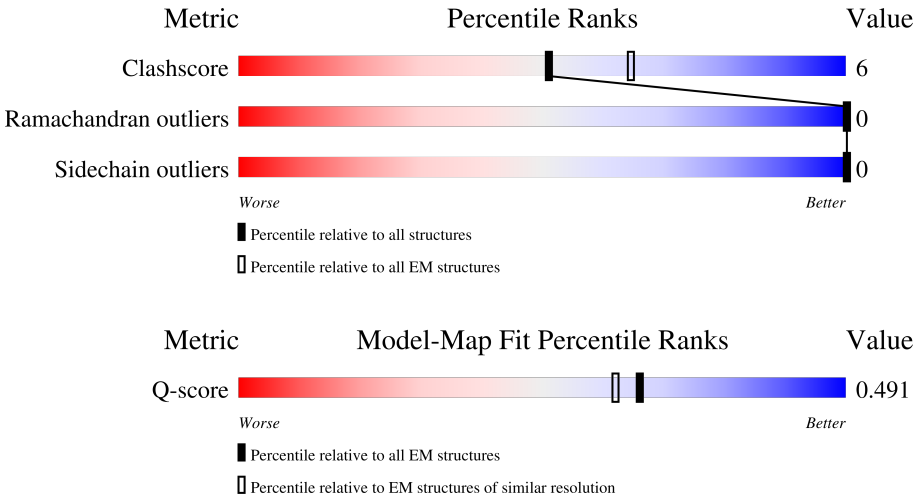
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 3.24 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	14594 (2.74 - 3.74)

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	D	217	43% 7% 50%
1	F	217	45% 5% 50%
1	H	217	43% 7% 50%
2	E	265	44% • 54%

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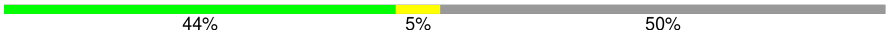
Mol	Chain	Length	Quality of chain
2	G	265	
2	I	265	
3	A	468	
3	B	468	
3	C	468	
4	J	216	
4	L	216	
4	N	216	
5	Q	216	
5	S	216	
5	U	216	
6	K	266	
6	M	266	
6	O	266	
7	R	270	
7	T	270	
7	V	270	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24051 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 Monoclonal Antibody RVA122 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	109	Total	C	N	O	S	0	0
			816	510	138	166	2		
1	F	109	Total	C	N	O	S	0	0
			816	510	138	166	2		
1	H	109	Total	C	N	O	S	0	0
			816	510	138	166	2		

- Molecule 2 is a protein called Monoclonal Antibody RVA122 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	122	Total	C	N	O	S	0	0
			952	607	152	189	4		
2	G	122	Total	C	N	O	S	0	0
			952	607	152	189	4		
2	I	122	Total	C	N	O	S	0	0
			952	607	152	189	4		

- Molecule 3 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	349	Total	C	N	O	S	0	0
			2723	1728	473	496	26		
3	B	349	Total	C	N	O	S	0	0
			2723	1728	473	496	26		
3	C	349	Total	C	N	O	S	0	0
			2723	1728	473	496	26		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	GLY	-	expression tag	UNP P08667
A	422	TRP	-	expression tag	UNP P08667
A	423	SER	-	expression tag	UNP P08667

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Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP P08667
A	425	PRO	-	expression tag	UNP P08667
A	426	GLN	-	expression tag	UNP P08667
A	427	PHE	-	expression tag	UNP P08667
A	428	GLU	-	expression tag	UNP P08667
A	429	LYS	-	expression tag	UNP P08667
A	430	GLY	-	expression tag	UNP P08667
A	431	GLY	-	expression tag	UNP P08667
A	432	GLY	-	expression tag	UNP P08667
A	433	SER	-	expression tag	UNP P08667
A	434	GLY	-	expression tag	UNP P08667
A	435	GLY	-	expression tag	UNP P08667
A	436	GLY	-	expression tag	UNP P08667
A	437	SER	-	expression tag	UNP P08667
A	438	GLY	-	expression tag	UNP P08667
A	439	GLY	-	expression tag	UNP P08667
A	440	GLY	-	expression tag	UNP P08667
A	441	SER	-	expression tag	UNP P08667
A	442	TRP	-	expression tag	UNP P08667
A	443	SER	-	expression tag	UNP P08667
A	444	HIS	-	expression tag	UNP P08667
A	445	PRO	-	expression tag	UNP P08667
A	446	GLN	-	expression tag	UNP P08667
A	447	PHE	-	expression tag	UNP P08667
A	448	GLU	-	expression tag	UNP P08667
A	449	LYS	-	expression tag	UNP P08667
A	450	GLY	-	expression tag	UNP P08667
A	451	SER	-	expression tag	UNP P08667
A	452	GLY	-	expression tag	UNP P08667
A	453	SER	-	expression tag	UNP P08667
A	454	GLY	-	expression tag	UNP P08667
A	455	LEU	-	expression tag	UNP P08667
A	456	ASN	-	expression tag	UNP P08667
A	457	ASP	-	expression tag	UNP P08667
A	458	ILE	-	expression tag	UNP P08667
A	459	PHE	-	expression tag	UNP P08667
A	460	GLU	-	expression tag	UNP P08667
A	461	ALA	-	expression tag	UNP P08667
A	462	GLN	-	expression tag	UNP P08667
A	463	LYS	-	expression tag	UNP P08667
A	464	ILE	-	expression tag	UNP P08667
A	465	GLU	-	expression tag	UNP P08667

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Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TRP	-	expression tag	UNP P08667
A	467	HIS	-	expression tag	UNP P08667
A	468	GLU	-	expression tag	UNP P08667
B	421	GLY	-	expression tag	UNP P08667
B	422	TRP	-	expression tag	UNP P08667
B	423	SER	-	expression tag	UNP P08667
B	424	HIS	-	expression tag	UNP P08667
B	425	PRO	-	expression tag	UNP P08667
B	426	GLN	-	expression tag	UNP P08667
B	427	PHE	-	expression tag	UNP P08667
B	428	GLU	-	expression tag	UNP P08667
B	429	LYS	-	expression tag	UNP P08667
B	430	GLY	-	expression tag	UNP P08667
B	431	GLY	-	expression tag	UNP P08667
B	432	GLY	-	expression tag	UNP P08667
B	433	SER	-	expression tag	UNP P08667
B	434	GLY	-	expression tag	UNP P08667
B	435	GLY	-	expression tag	UNP P08667
B	436	GLY	-	expression tag	UNP P08667
B	437	SER	-	expression tag	UNP P08667
B	438	GLY	-	expression tag	UNP P08667
B	439	GLY	-	expression tag	UNP P08667
B	440	GLY	-	expression tag	UNP P08667
B	441	SER	-	expression tag	UNP P08667
B	442	TRP	-	expression tag	UNP P08667
B	443	SER	-	expression tag	UNP P08667
B	444	HIS	-	expression tag	UNP P08667
B	445	PRO	-	expression tag	UNP P08667
B	446	GLN	-	expression tag	UNP P08667
B	447	PHE	-	expression tag	UNP P08667
B	448	GLU	-	expression tag	UNP P08667
B	449	LYS	-	expression tag	UNP P08667
B	450	GLY	-	expression tag	UNP P08667
B	451	SER	-	expression tag	UNP P08667
B	452	GLY	-	expression tag	UNP P08667
B	453	SER	-	expression tag	UNP P08667
B	454	GLY	-	expression tag	UNP P08667
B	455	LEU	-	expression tag	UNP P08667
B	456	ASN	-	expression tag	UNP P08667
B	457	ASP	-	expression tag	UNP P08667
B	458	ILE	-	expression tag	UNP P08667
B	459	PHE	-	expression tag	UNP P08667

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Chain	Residue	Modelled	Actual	Comment	Reference
B	460	GLU	-	expression tag	UNP P08667
B	461	ALA	-	expression tag	UNP P08667
B	462	GLN	-	expression tag	UNP P08667
B	463	LYS	-	expression tag	UNP P08667
B	464	ILE	-	expression tag	UNP P08667
B	465	GLU	-	expression tag	UNP P08667
B	466	TRP	-	expression tag	UNP P08667
B	467	HIS	-	expression tag	UNP P08667
B	468	GLU	-	expression tag	UNP P08667
C	421	GLY	-	expression tag	UNP P08667
C	422	TRP	-	expression tag	UNP P08667
C	423	SER	-	expression tag	UNP P08667
C	424	HIS	-	expression tag	UNP P08667
C	425	PRO	-	expression tag	UNP P08667
C	426	GLN	-	expression tag	UNP P08667
C	427	PHE	-	expression tag	UNP P08667
C	428	GLU	-	expression tag	UNP P08667
C	429	LYS	-	expression tag	UNP P08667
C	430	GLY	-	expression tag	UNP P08667
C	431	GLY	-	expression tag	UNP P08667
C	432	GLY	-	expression tag	UNP P08667
C	433	SER	-	expression tag	UNP P08667
C	434	GLY	-	expression tag	UNP P08667
C	435	GLY	-	expression tag	UNP P08667
C	436	GLY	-	expression tag	UNP P08667
C	437	SER	-	expression tag	UNP P08667
C	438	GLY	-	expression tag	UNP P08667
C	439	GLY	-	expression tag	UNP P08667
C	440	GLY	-	expression tag	UNP P08667
C	441	SER	-	expression tag	UNP P08667
C	442	TRP	-	expression tag	UNP P08667
C	443	SER	-	expression tag	UNP P08667
C	444	HIS	-	expression tag	UNP P08667
C	445	PRO	-	expression tag	UNP P08667
C	446	GLN	-	expression tag	UNP P08667
C	447	PHE	-	expression tag	UNP P08667
C	448	GLU	-	expression tag	UNP P08667
C	449	LYS	-	expression tag	UNP P08667
C	450	GLY	-	expression tag	UNP P08667
C	451	SER	-	expression tag	UNP P08667
C	452	GLY	-	expression tag	UNP P08667
C	453	SER	-	expression tag	UNP P08667

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Chain	Residue	Modelled	Actual	Comment	Reference
C	454	GLY	-	expression tag	UNP P08667
C	455	LEU	-	expression tag	UNP P08667
C	456	ASN	-	expression tag	UNP P08667
C	457	ASP	-	expression tag	UNP P08667
C	458	ILE	-	expression tag	UNP P08667
C	459	PHE	-	expression tag	UNP P08667
C	460	GLU	-	expression tag	UNP P08667
C	461	ALA	-	expression tag	UNP P08667
C	462	GLN	-	expression tag	UNP P08667
C	463	LYS	-	expression tag	UNP P08667
C	464	ILE	-	expression tag	UNP P08667
C	465	GLU	-	expression tag	UNP P08667
C	466	TRP	-	expression tag	UNP P08667
C	467	HIS	-	expression tag	UNP P08667
C	468	GLU	-	expression tag	UNP P08667

- Molecule 4 is a protein called Monoclonal Antibody 4H3 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	108	Total	C	N	O	S	0	0
			799	496	140	161	2		
4	L	108	Total	C	N	O	S	0	0
			799	496	140	161	2		
4	N	108	Total	C	N	O	S	0	0
			799	496	140	161	2		

- Molecule 5 is a protein called Monoclonal Antibody 4C12 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	108	Total	C	N	O	S	0	0
			793	491	137	163	2		
5	U	108	Total	C	N	O	S	0	0
			793	491	137	163	2		
5	Q	108	Total	C	N	O	S	0	0
			793	491	137	163	2		

- Molecule 6 is a protein called Monoclonal Antibody 4H3 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	120	Total	C	N	O	S	0	0
			953	605	159	182	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	120	Total	C	N	O	S	0	0
			953	605	159	182	7		
6	O	120	Total	C	N	O	S	0	0
			953	605	159	182	7		

- Molecule 7 is a protein called Monoclonal Antibody 4C12 Heavy Chain.

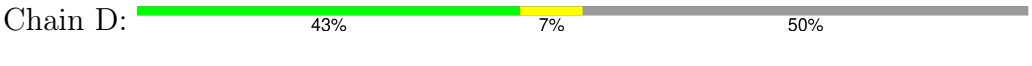
Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	125	Total	C	N	O	S	0	0
			981	629	160	190	2		
7	T	125	Total	C	N	O	S	0	0
			981	629	160	190	2		
7	V	125	Total	C	N	O	S	0	0
			981	629	160	190	2		

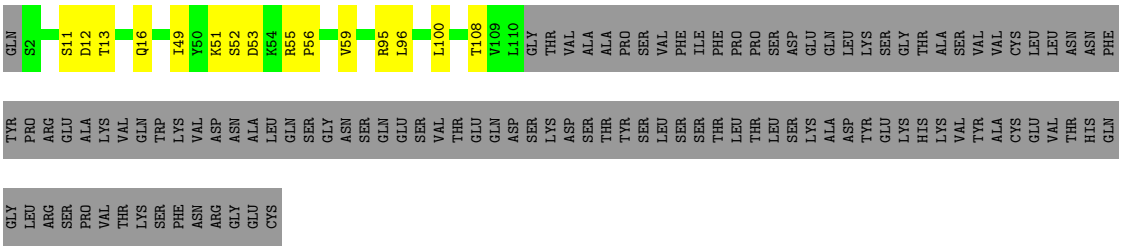
3 Residue-property plots (i)

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: Monoclonal Antibody RVA122 Light Chain

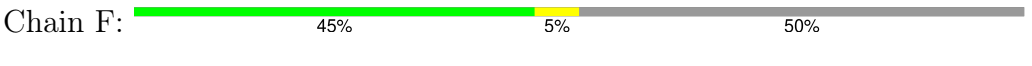
Chain D:

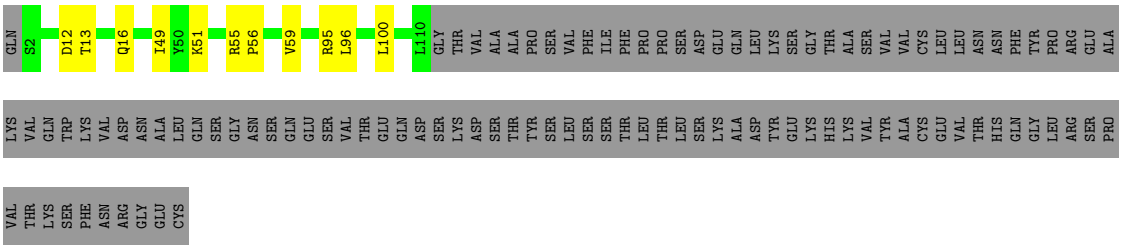




• Molecule 1: Monoclonal Antibody RVA122 Light Chain

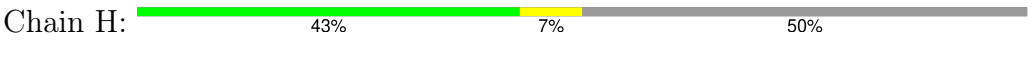
Chain F:

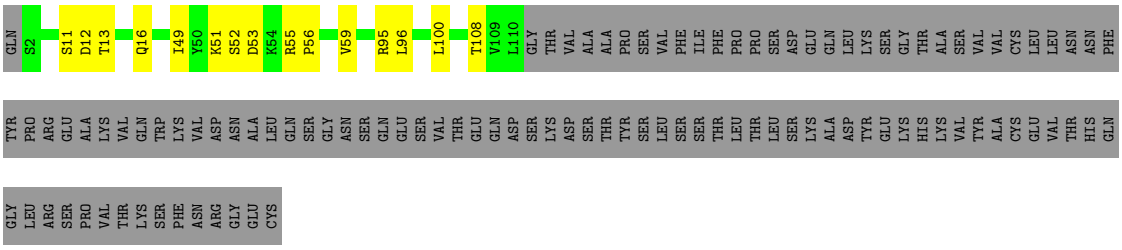




• Molecule 1: Monoclonal Antibody RVA122 Light Chain

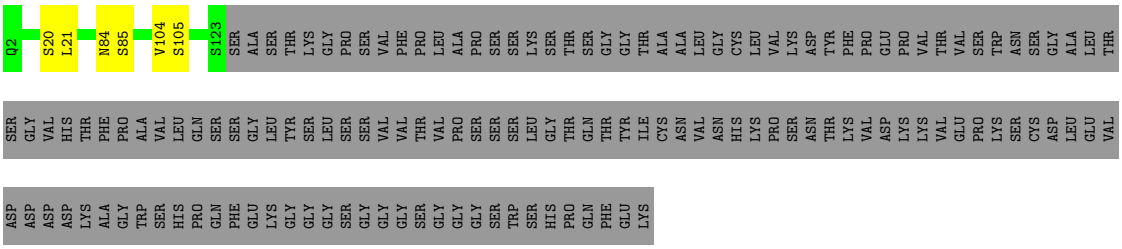
Chain H:





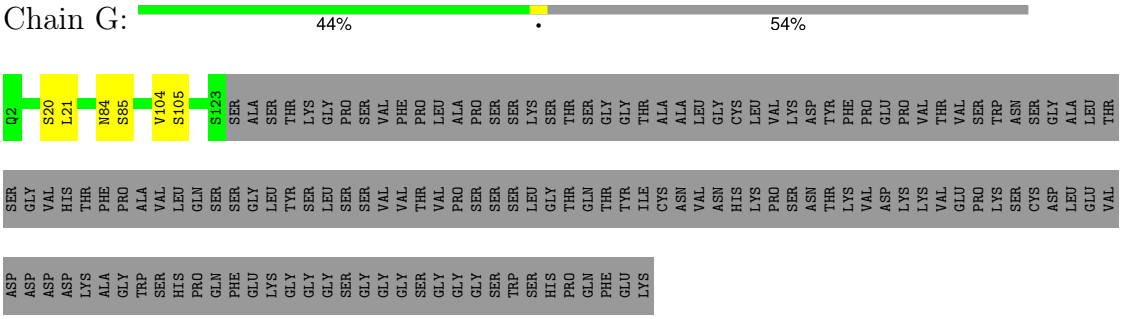
• Molecule 2: Monoclonal Antibody RVA122 Heavy Chain

Chain E:



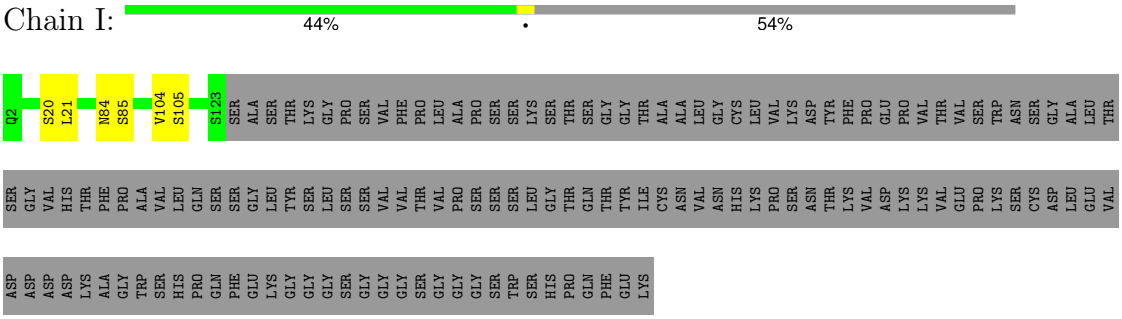
• Molecule 2: Monoclonal Antibody RVA122 Heavy Chain

Chain G:



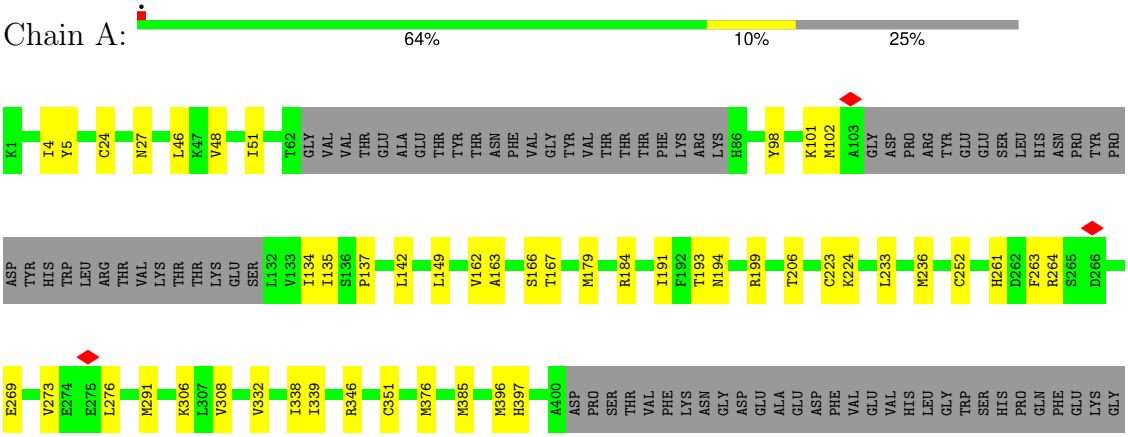
• Molecule 2: Monoclonal Antibody RVA122 Heavy Chain

Chain I:



• Molecule 3: Glycoprotein

Chain A:

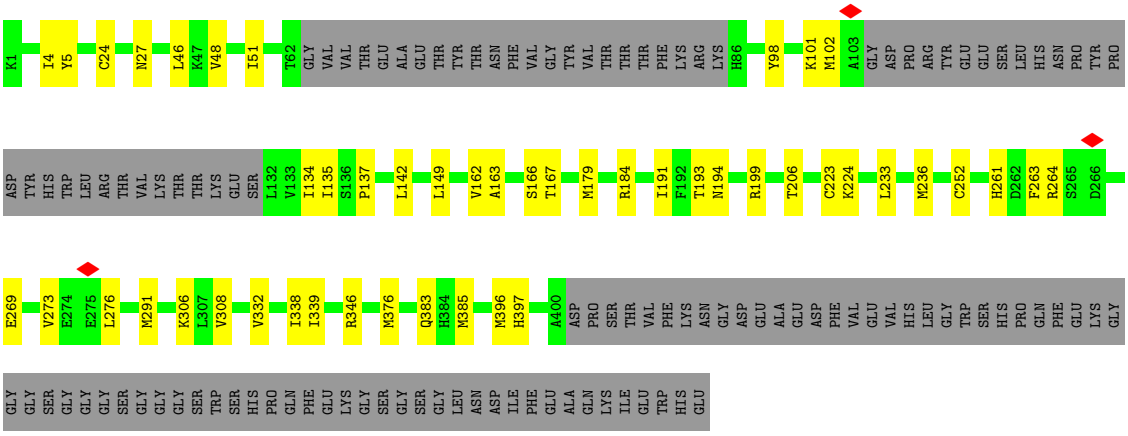




• Molecule 3: Glycoprotein

Chain B:

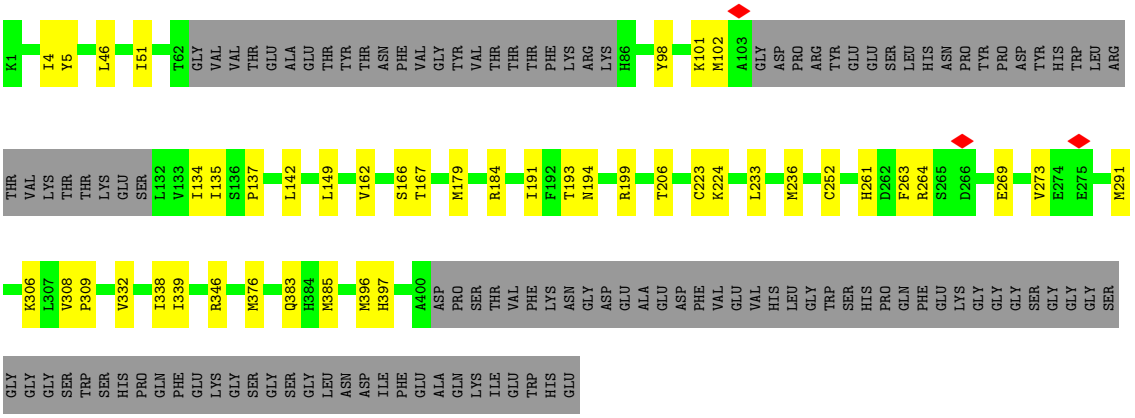




• Molecule 3: Glycoprotein

Chain C:

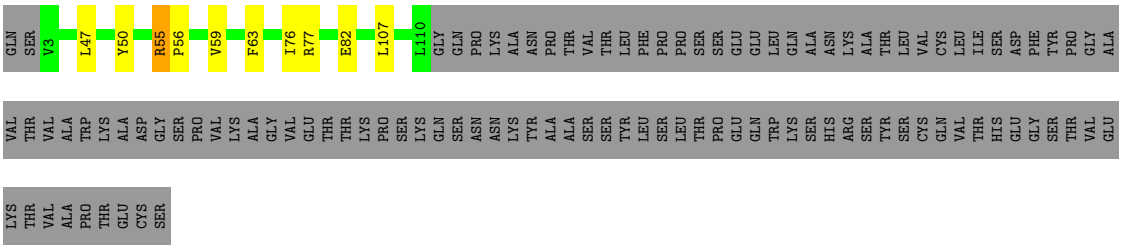




• Molecule 4: Monoclonal Antibody 4H3 Light Chain

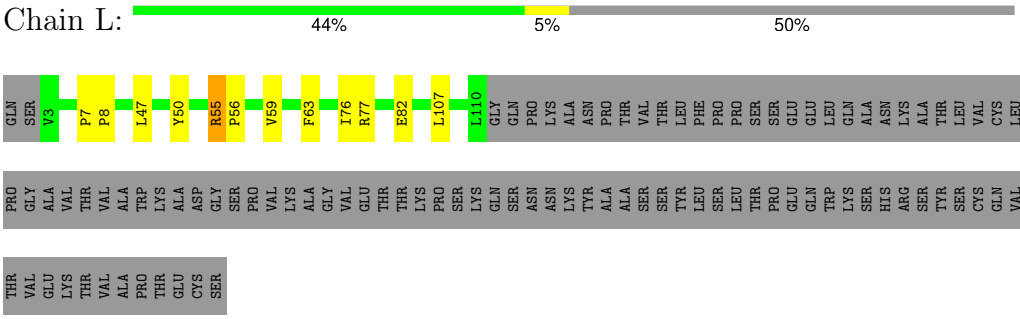
Chain J:





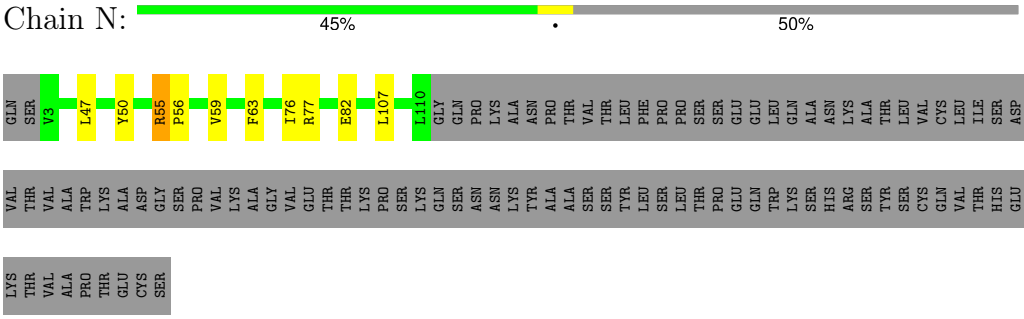
• Molecule 4: Monoclonal Antibody 4H3 Light Chain

Chain L:



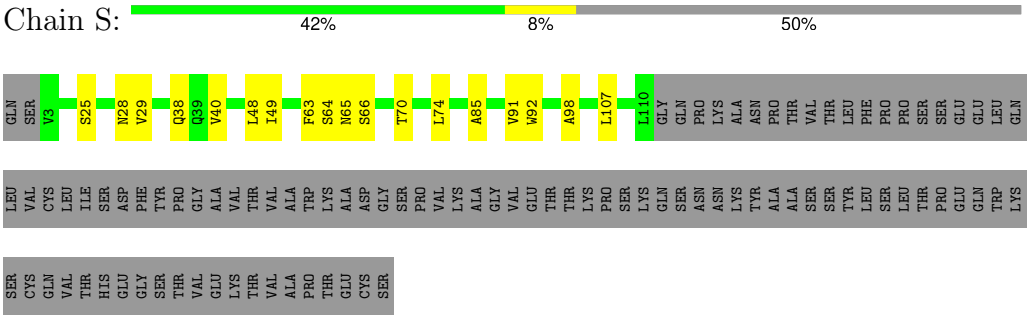
• Molecule 4: Monoclonal Antibody 4H3 Light Chain

Chain N:



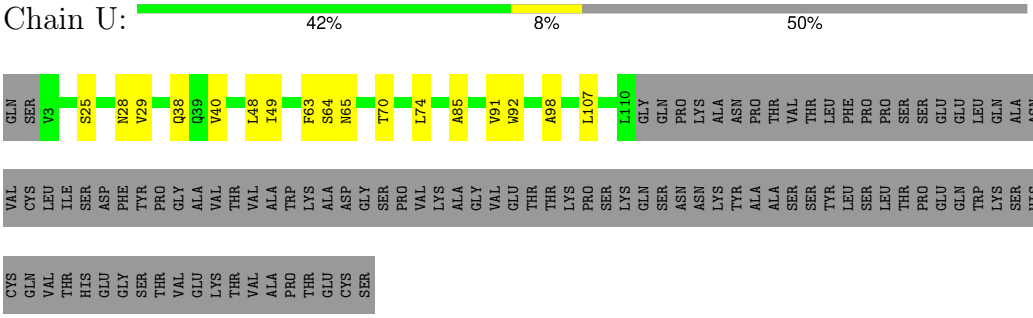
• Molecule 5: Monoclonal Antibody 4C12 Light Chain

Chain S:



• Molecule 5: Monoclonal Antibody 4C12 Light Chain

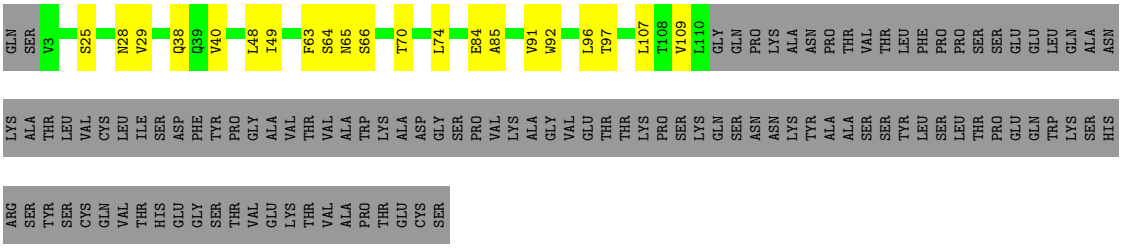
Chain U:



• Molecule 5: Monoclonal Antibody 4C12 Light Chain

Chain Q:

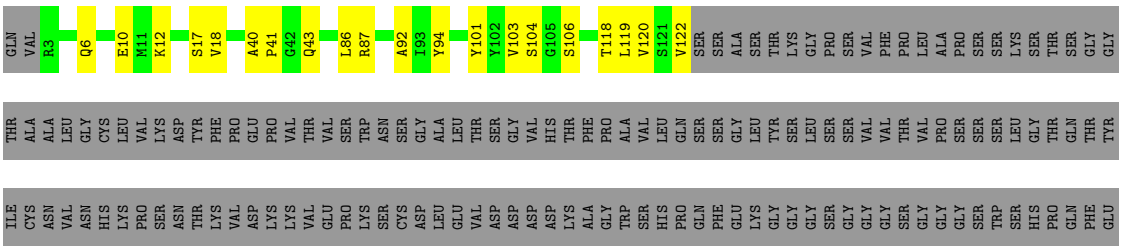




• Molecule 6: Monoclonal Antibody 4H3 Heavy Chain

Chain K:

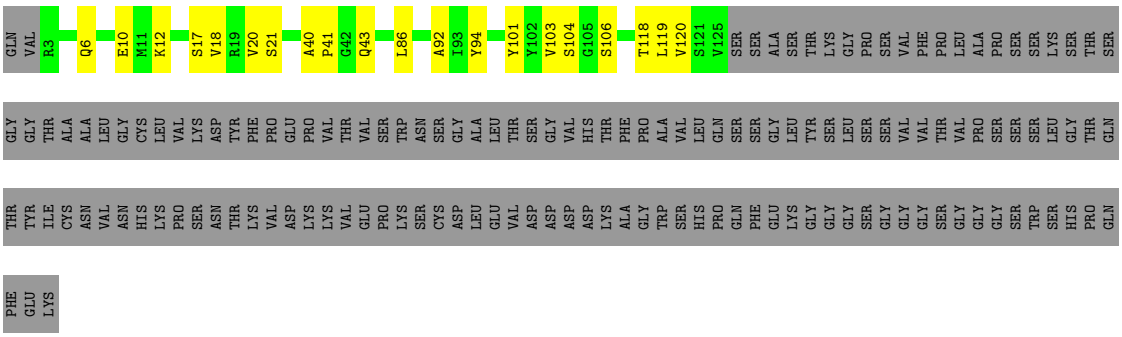




• Molecule 6: Monoclonal Antibody 4H3 Heavy Chain

Chain M:

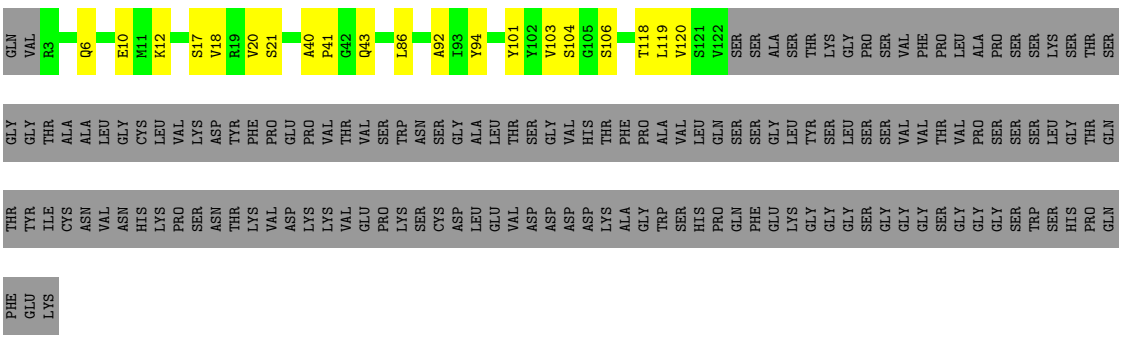




• Molecule 6: Monoclonal Antibody 4H3 Heavy Chain

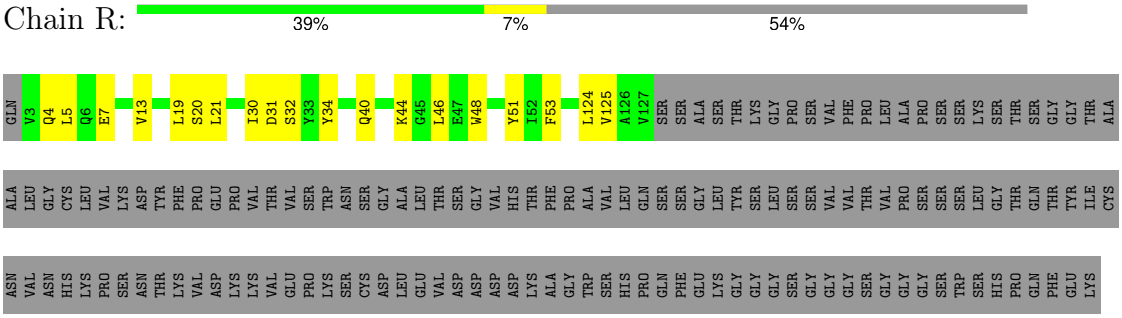
Chain O:





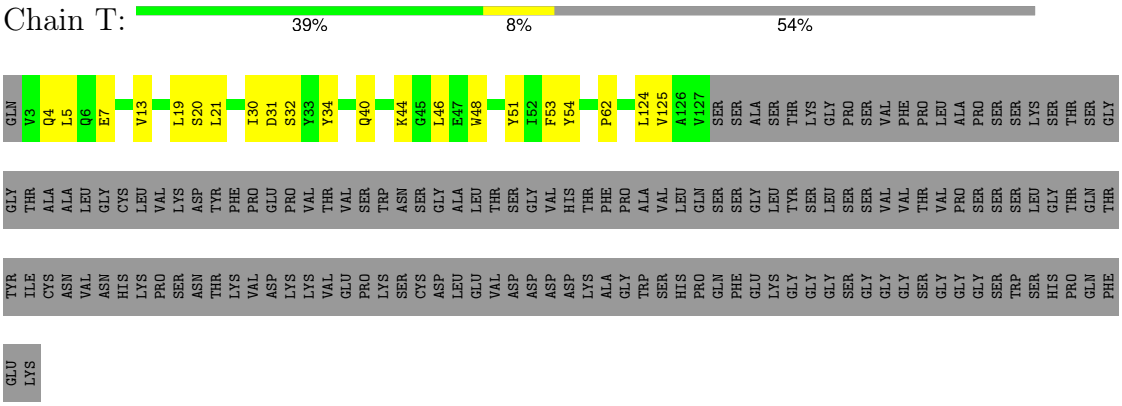
• Molecule 7: Monoclonal Antibody 4C12 Heavy Chain

Chain R:



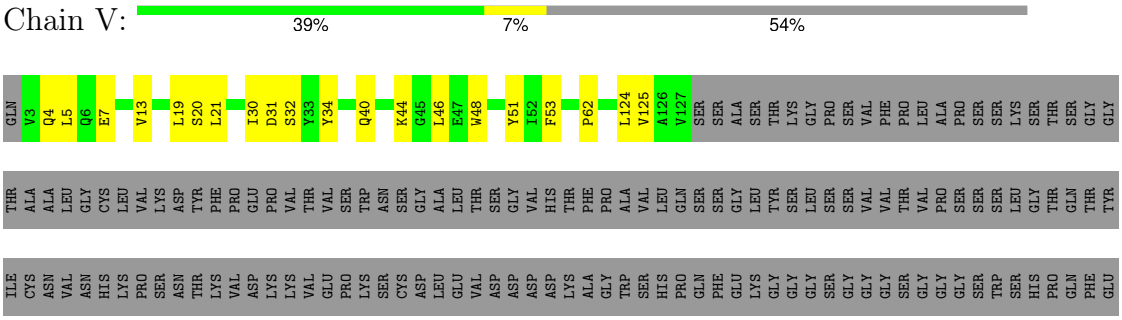
• Molecule 7: Monoclonal Antibody 4C12 Heavy Chain

Chain T:



• Molecule 7: Monoclonal Antibody 4C12 Heavy Chain

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	262318	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.623	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	D	0.13	0/836	0.27	0/1137
1	F	0.13	0/836	0.27	0/1137
1	H	0.13	0/836	0.27	0/1137
2	E	0.14	0/979	0.22	0/1338
2	G	0.14	0/979	0.22	0/1338
2	I	0.14	0/979	0.22	0/1338
3	A	0.20	0/2789	0.34	0/3776
3	B	0.20	0/2789	0.34	0/3776
3	C	0.20	0/2789	0.34	0/3776
4	J	0.15	0/819	0.34	0/1117
4	L	0.15	0/819	0.34	0/1117
4	N	0.16	0/819	0.34	0/1117
5	Q	0.18	0/812	0.30	0/1112
5	S	0.17	0/812	0.30	0/1112
5	U	0.18	0/812	0.30	0/1112
6	K	0.15	0/980	0.30	0/1331
6	M	0.15	0/980	0.31	0/1331
6	O	0.15	0/980	0.30	0/1331
7	R	0.16	0/1011	0.30	0/1382
7	T	0.16	0/1011	0.30	0/1382
7	V	0.16	0/1011	0.30	0/1382
All	All	0.17	0/24678	0.31	0/33579

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	D	0	1
1	F	0	1
1	H	0	1
3	A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	3
3	C	0	3
4	J	0	2
4	L	0	2
4	N	0	2
All	All	0	18

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	184	ARG	Sidechain
3	A	264	ARG	Sidechain
3	A	346	ARG	Sidechain
1	D	55	ARG	Sidechain
1	F	55	ARG	Sidechain

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	D	816	0	778	8	0
1	F	816	0	778	6	0
1	H	816	0	778	8	0
2	E	952	0	898	3	0
2	G	952	0	898	3	0
2	I	952	0	898	3	0
3	A	2723	0	2700	31	0
3	B	2723	0	2700	30	0
3	C	2723	0	2700	28	0
4	J	799	0	761	8	0
4	L	799	0	761	8	0
4	N	799	0	761	8	0
5	Q	793	0	750	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	793	0	750	14	0
5	U	793	0	750	13	0
6	K	953	0	894	13	0
6	M	953	0	894	13	0
6	O	953	0	894	13	0
7	R	981	0	924	14	0
7	T	981	0	924	16	0
7	V	981	0	924	16	0
All	All	24051	0	23115	261	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 6.

The worst 5 of 261 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:A:291:MET:HE1	3:B:385:MET:HE3	1.74	0.69
3:B:291:MET:HE1	3:C:385:MET:HE3	1.75	0.69
3:B:135:ILE:HG22	3:B:137:PRO:HD2	1.78	0.66
3:C:135:ILE:HG22	3:C:137:PRO:HD2	1.78	0.66
3:A:135:ILE:HG22	3:A:137:PRO:HD2	1.78	0.66

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	D	107/217 (49%)	103 (96%)	4 (4%)	0	100	100
1	F	107/217 (49%)	103 (96%)	4 (4%)	0	100	100
1	H	107/217 (49%)	103 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	120/265 (45%)	119 (99%)	1 (1%)	0	100	100
2	G	120/265 (45%)	119 (99%)	1 (1%)	0	100	100
2	I	120/265 (45%)	119 (99%)	1 (1%)	0	100	100
3	A	343/468 (73%)	339 (99%)	4 (1%)	0	100	100
3	B	343/468 (73%)	339 (99%)	4 (1%)	0	100	100
3	C	343/468 (73%)	339 (99%)	4 (1%)	0	100	100
4	J	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
4	L	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
4	N	106/216 (49%)	101 (95%)	5 (5%)	0	100	100
5	Q	106/216 (49%)	106 (100%)	0	0	100	100
5	S	106/216 (49%)	106 (100%)	0	0	100	100
5	U	106/216 (49%)	106 (100%)	0	0	100	100
6	K	118/266 (44%)	115 (98%)	3 (2%)	0	100	100
6	M	118/266 (44%)	115 (98%)	3 (2%)	0	100	100
6	O	118/266 (44%)	115 (98%)	3 (2%)	0	100	100
7	R	123/270 (46%)	123 (100%)	0	0	100	100
7	T	123/270 (46%)	122 (99%)	1 (1%)	0	100	100
7	V	123/270 (46%)	122 (99%)	1 (1%)	0	100	100
All	All	3069/5754 (53%)	3016 (98%)	53 (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	D	90/186 (48%)	90 (100%)	0	100	100
1	F	90/186 (48%)	90 (100%)	0	100	100
1	H	90/186 (48%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	105/223 (47%)	105 (100%)	0	100	100
2	G	105/223 (47%)	105 (100%)	0	100	100
2	I	105/223 (47%)	105 (100%)	0	100	100
3	A	307/406 (76%)	307 (100%)	0	100	100
3	B	307/406 (76%)	307 (100%)	0	100	100
3	C	307/406 (76%)	307 (100%)	0	100	100
4	J	88/181 (49%)	88 (100%)	0	100	100
4	L	88/181 (49%)	88 (100%)	0	100	100
4	N	88/181 (49%)	88 (100%)	0	100	100
5	Q	88/181 (49%)	88 (100%)	0	100	100
5	S	88/181 (49%)	88 (100%)	0	100	100
5	U	88/181 (49%)	88 (100%)	0	100	100
6	K	99/220 (45%)	99 (100%)	0	100	100
6	M	99/220 (45%)	99 (100%)	0	100	100
6	O	99/220 (45%)	99 (100%)	0	100	100
7	R	107/227 (47%)	107 (100%)	0	100	100
7	T	107/227 (47%)	107 (100%)	0	100	100
7	V	107/227 (47%)	107 (100%)	0	100	100
All	All	2652/4872 (54%)	2652 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	54	GLN
7	T	4	GLN
3	C	37	ASN
6	O	39	GLN
3	B	261	HIS

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 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.

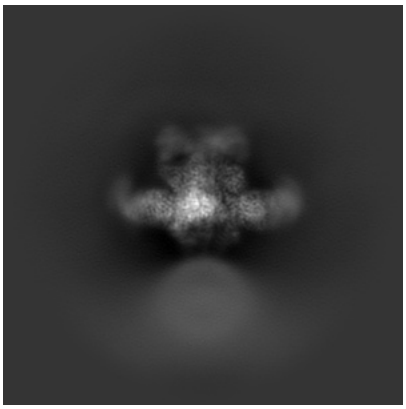
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-75813. These allow visual inspection of the internal detail of the map and identification of artifacts.

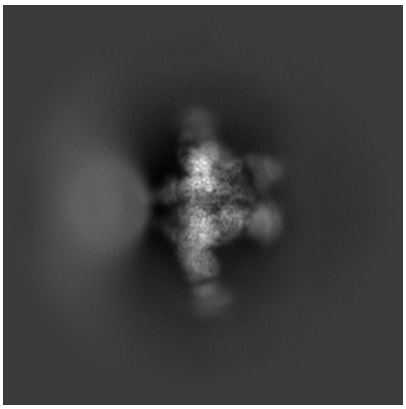
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

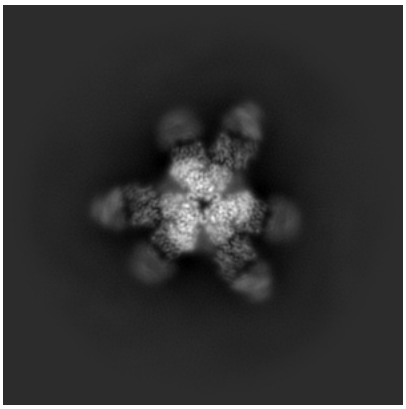
6.1.1 Primary map



X

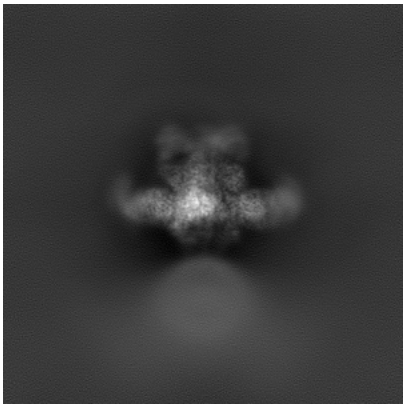


Y



Z

6.1.2 Raw map



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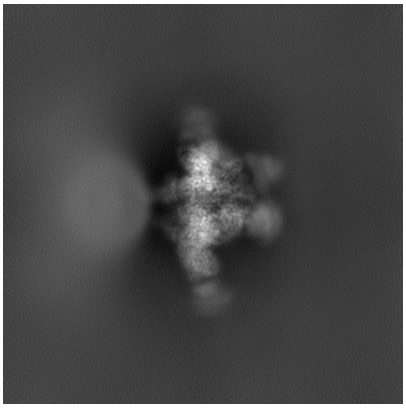
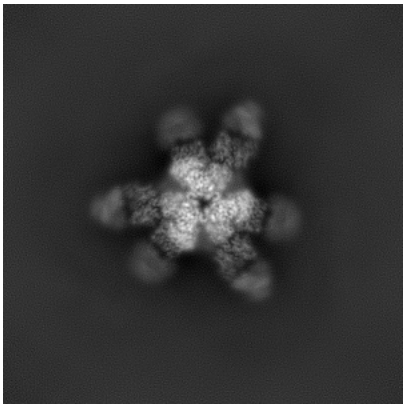


Y

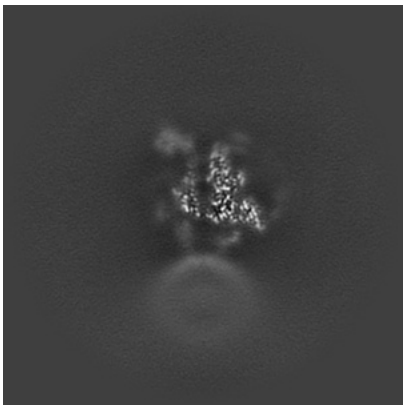


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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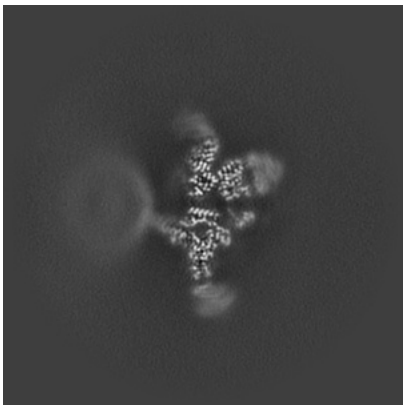
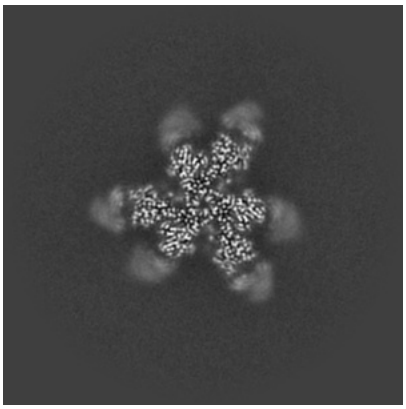
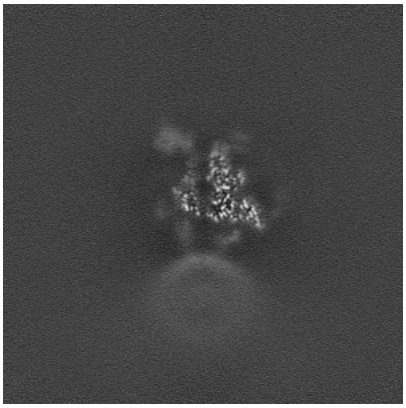


Y Index: 200

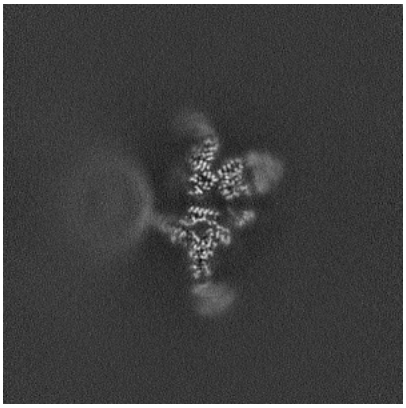


Z Index: 200

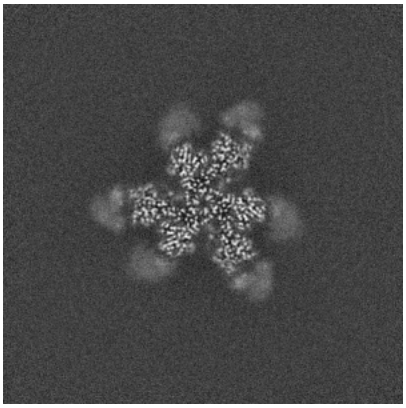
6.2.2 Raw map



X Index: 200



Y Index: 200

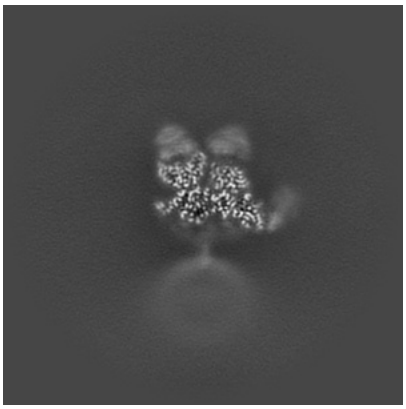


Z Index: 200

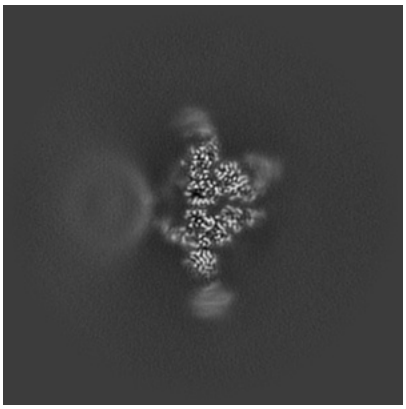
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

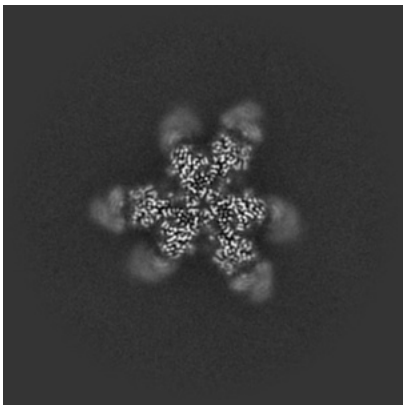
6.3.1 Primary map



X Index: 188

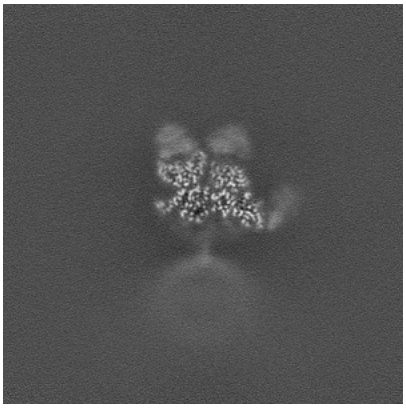


Y Index: 193

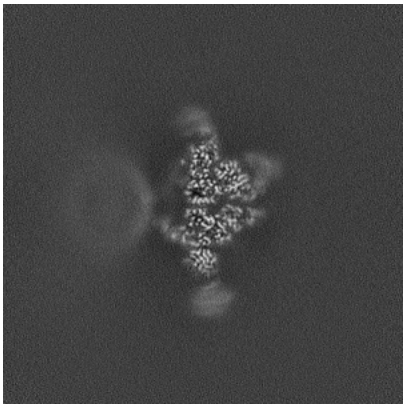


Z Index: 201

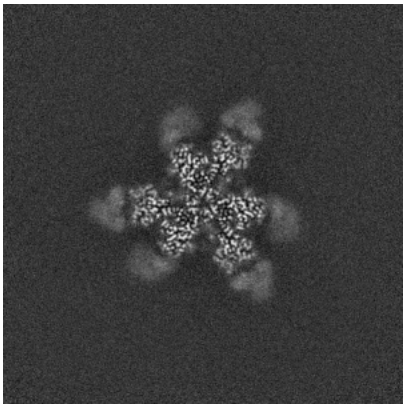
6.3.2 Raw map



X Index: 188



Y Index: 193

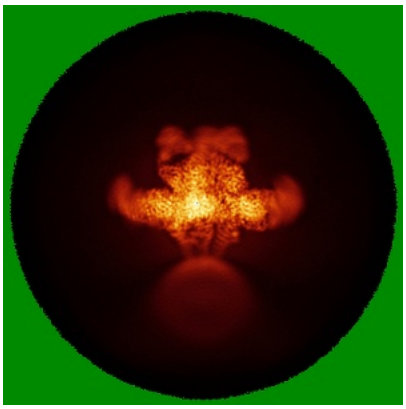


Z Index: 201

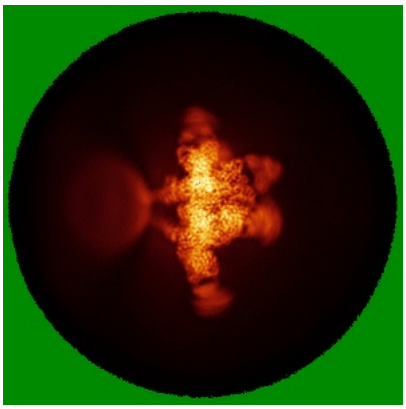
The images above show the largest variance slices of the map in three orthogonal directions.

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

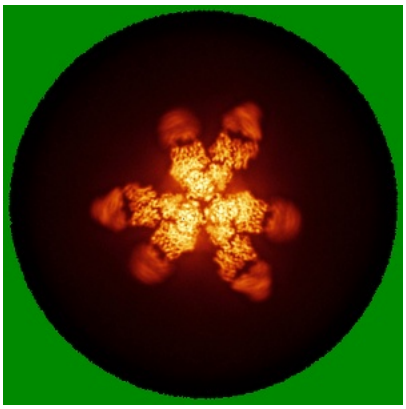
6.4.1 Primary map



X

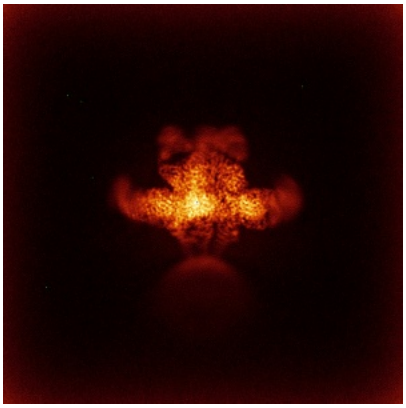


Y

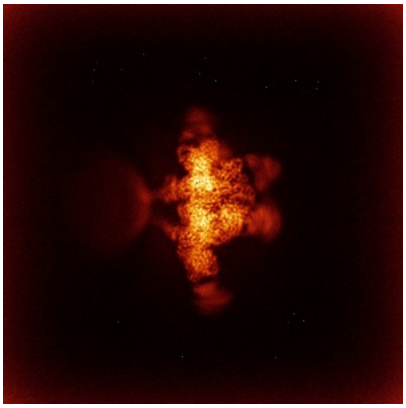


Z

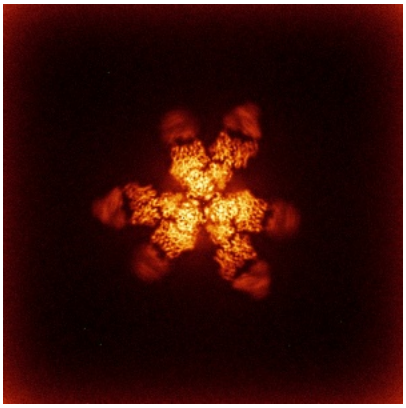
6.4.2 Raw map



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 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

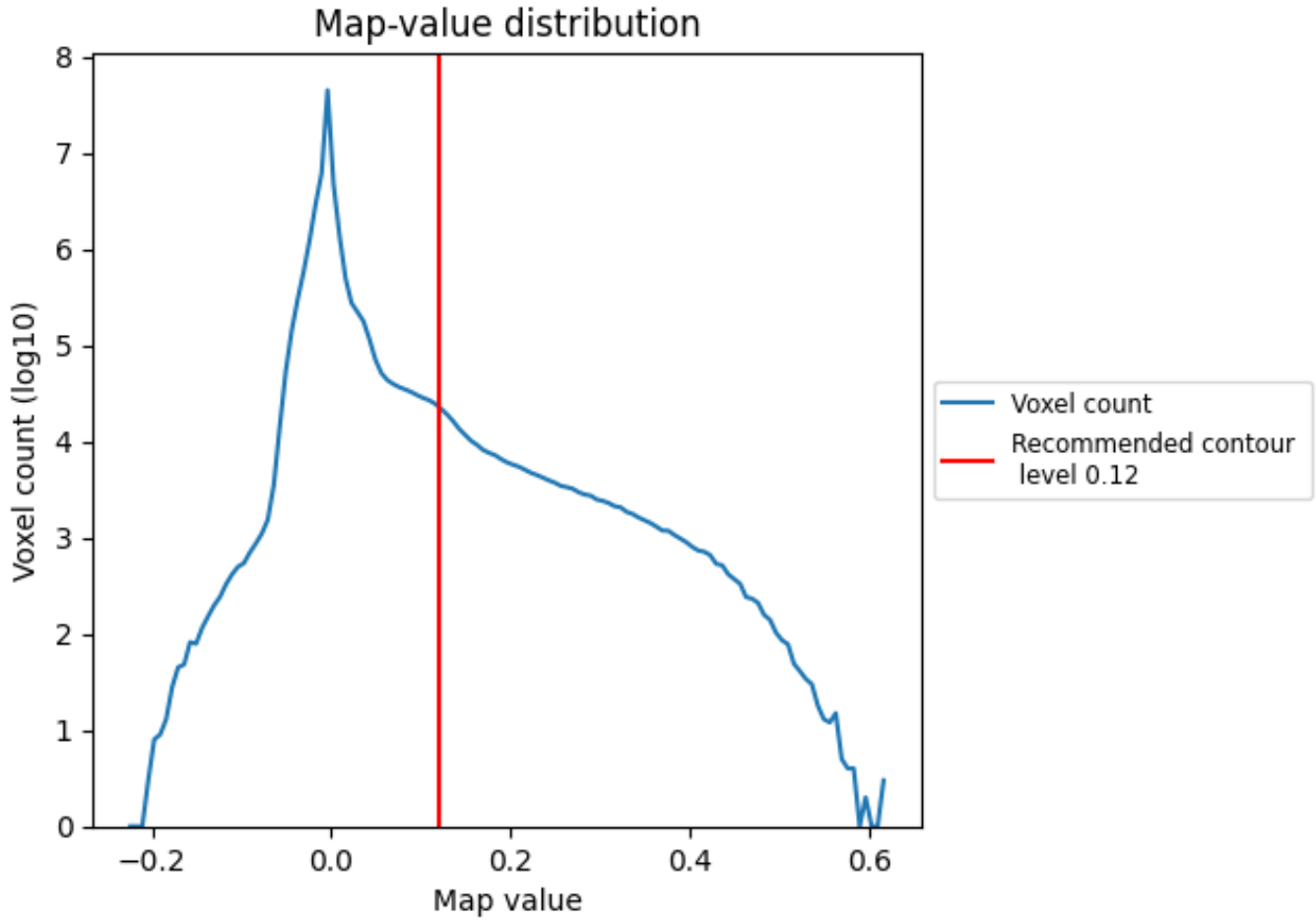
6.6 Mask visualisation (i)

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

7 Map analysis

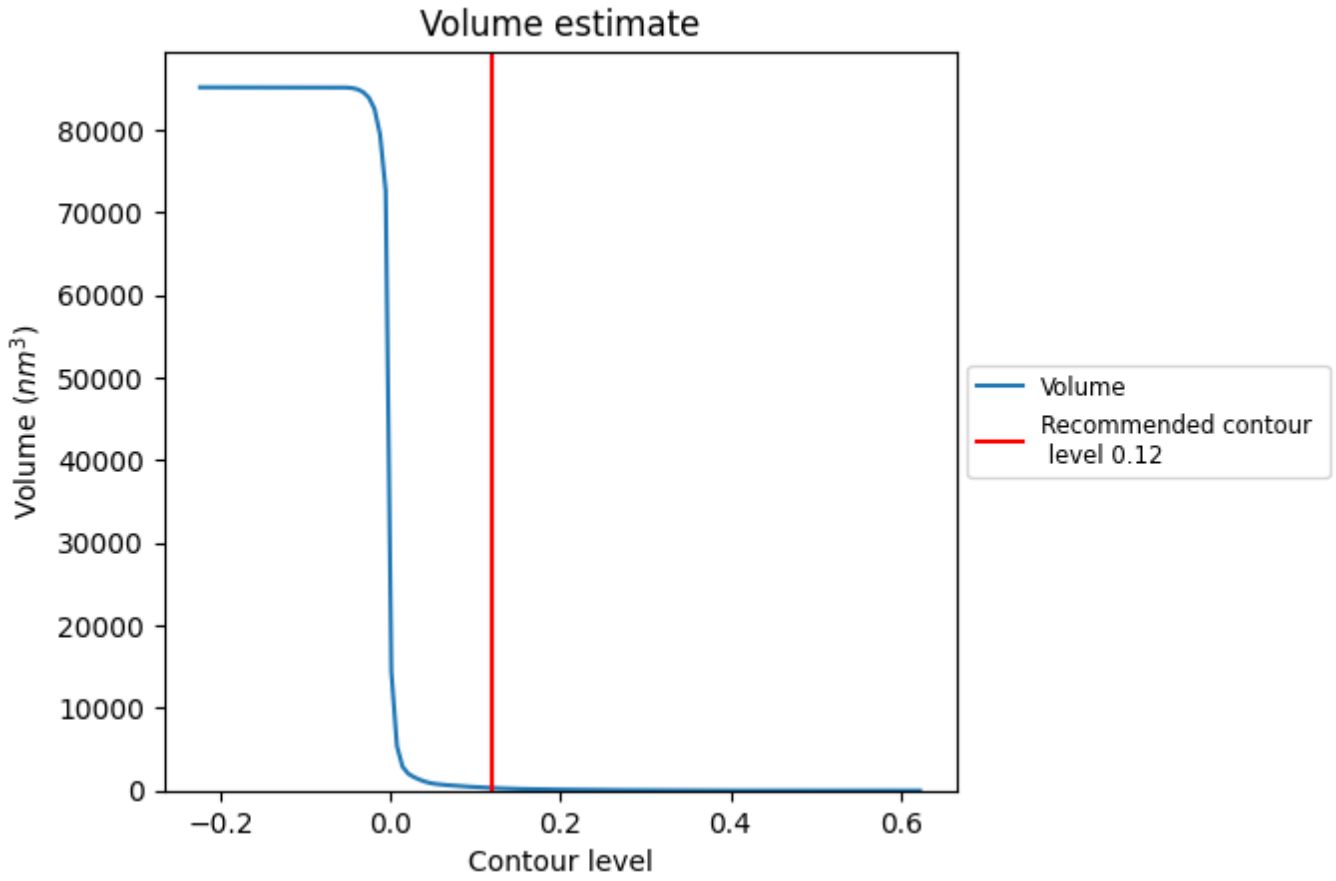
This section contains the results of statistical analysis of the map.

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.

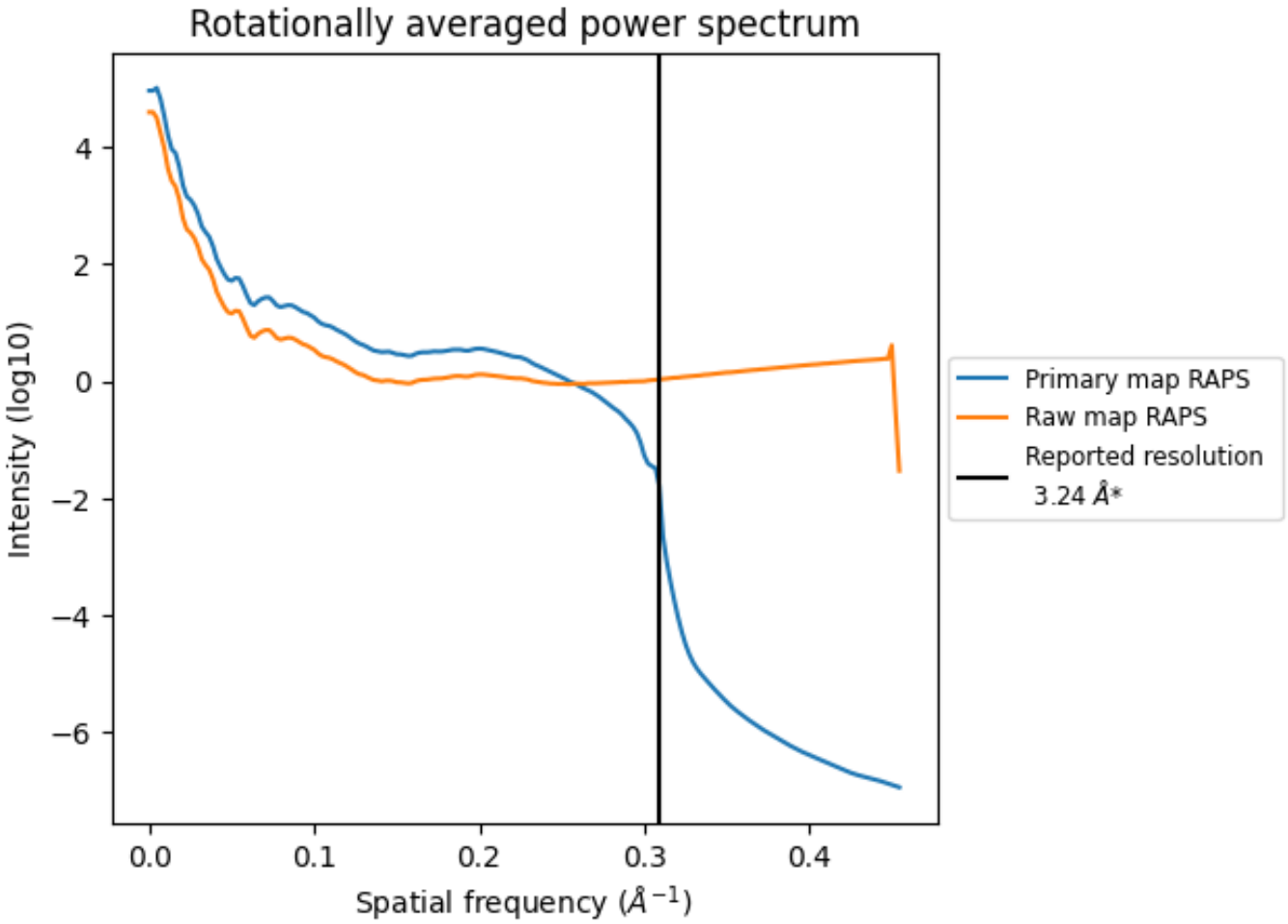
7.2 Volume estimate (i)



The volume at the recommended contour level is 313 nm^3; this corresponds to an approximate mass of 283 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)

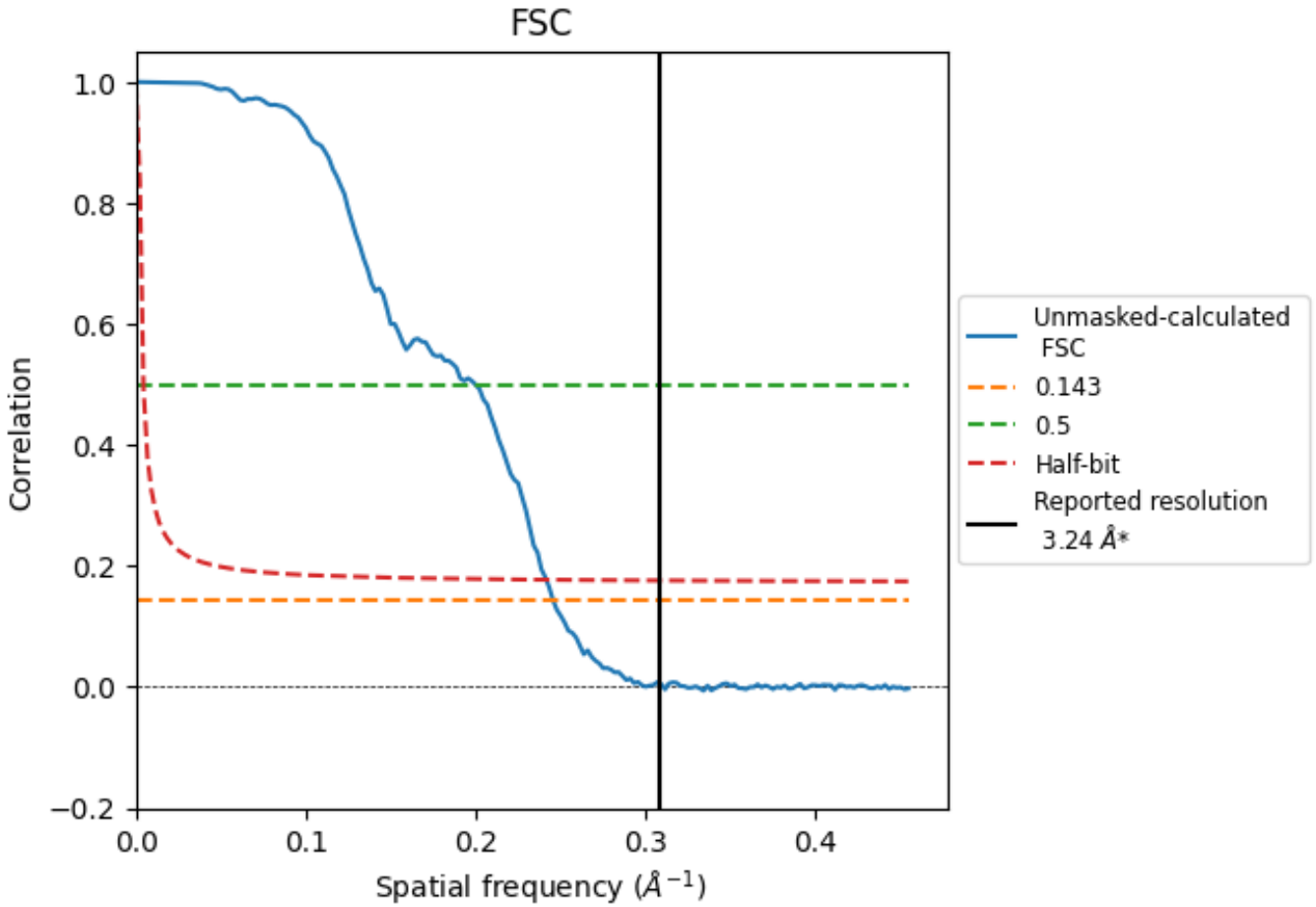


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8.2 Resolution estimates (i)

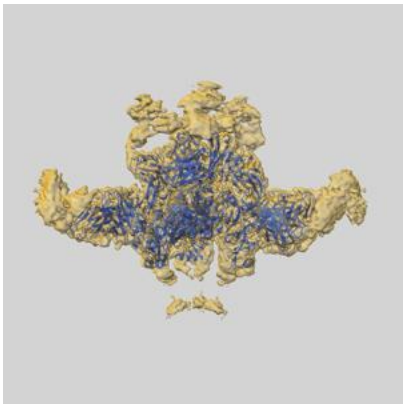
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	5.01	4.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.24 by more than 10 %

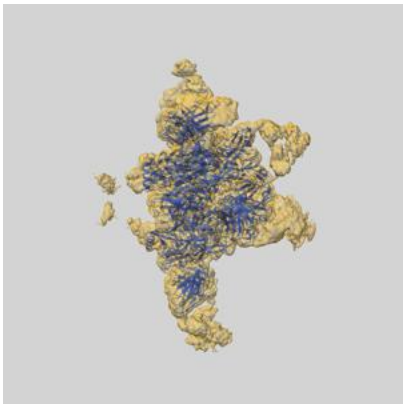
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-75813 and PDB model 11LQ. Per-residue inclusion information can be found in section 3 on page 10.

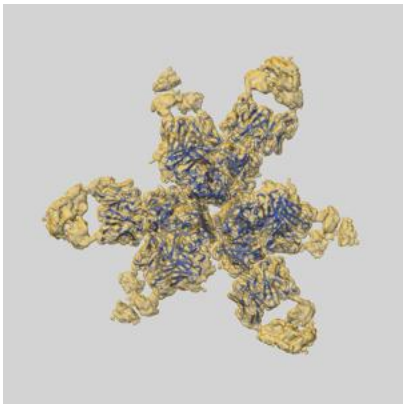
9.1 Map-model overlay



X



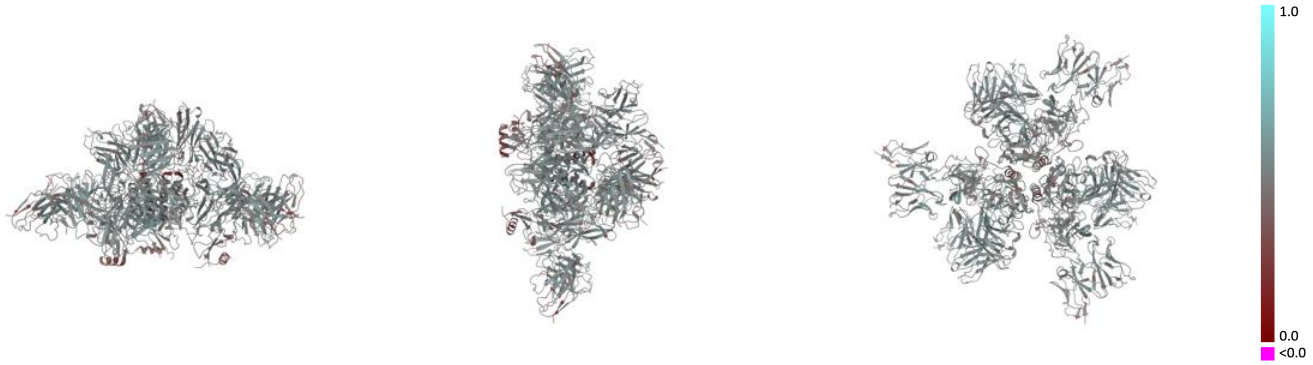
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

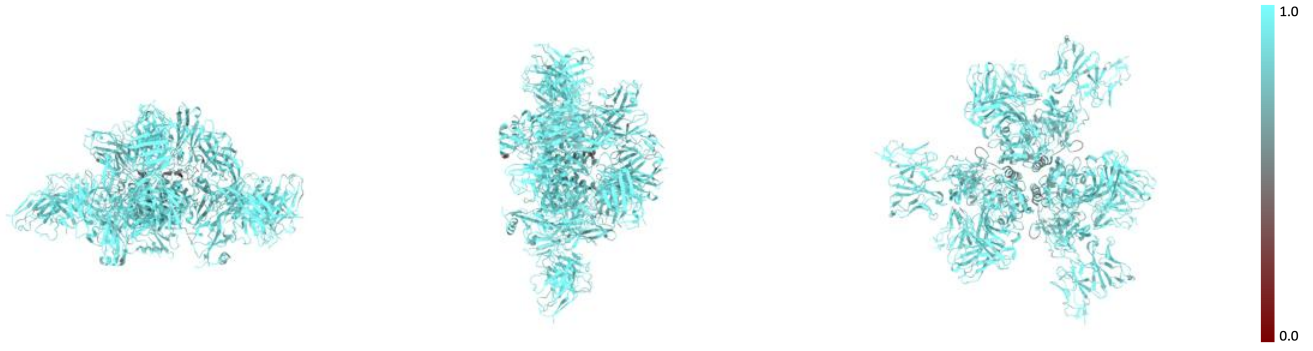
9.2 Q-score mapped to coordinate model (i)



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.

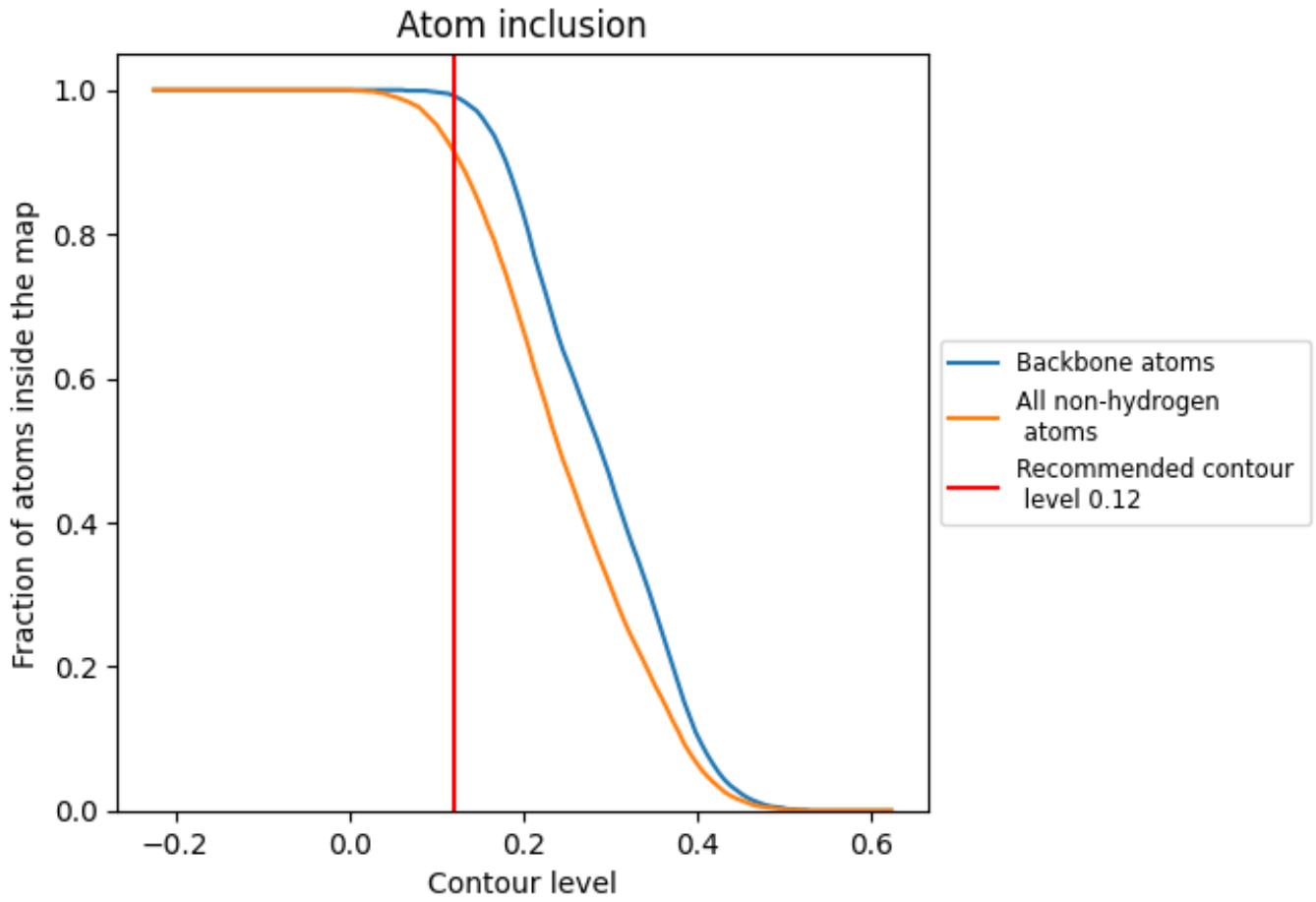
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.4910
A	0.8840	0.4830
B	0.8830	0.4830
C	0.8850	0.4810
D	0.9010	0.4860
E	0.9450	0.5060
F	0.8980	0.4840
G	0.9470	0.5010
H	0.9030	0.4820
I	0.9440	0.5000
J	0.9140	0.4650
K	0.9250	0.4940
L	0.9130	0.4650
M	0.9250	0.4930
N	0.9110	0.4620
O	0.9200	0.4890
Q	0.9500	0.5130
R	0.9500	0.5070
S	0.9500	0.5160
T	0.9480	0.5080
U	0.9510	0.5160
V	0.9500	0.5090

