Full wwPDB EM Validation Report (i)

Sep 20, 2026 – 12:20 PM EDT

PDB ID	:	11LR / pdb_000011lr
EMDB ID	:	EMD-75814
Title	:	Human monoclonal antibody 8C5 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	:	3.16 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

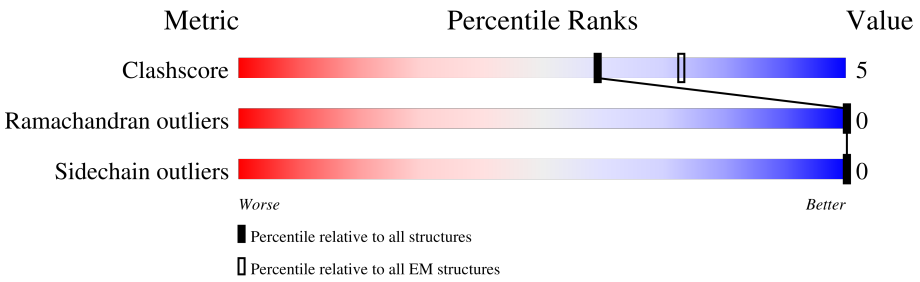
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

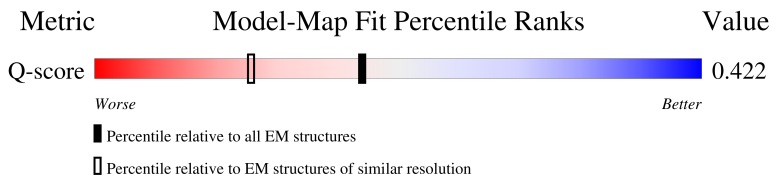
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.16 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	14474 (2.66 - 3.66)

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	E	265	38% 8% 54%
1	G	265	38% 8% 54%
1	I	265	38% 8% 54%
2	A	468	68% 11% 22%

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Mol	Chain	Length	Quality of chain
2	B	468	68% 10% 22%
2	C	468	68% 10% 22%
3	D	217	46% • 50%
3	F	217	46% • 50%
3	H	217	46% 5% 50%
4	J	216	45% 5% 50%
4	L	216	45% 6% 50%
4	N	216	45% 5% 50%
5	K	264	42% • 55%
5	M	264	42% • 55%
5	o	264	43% • 55%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19287 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 Heavy Chain.

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

- Molecule 2 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	367	2866	1815	500	525	26	0	0
2	B	367	2866	1815	500	525	26	0	0
2	C	367	2866	1815	500	525	26	0	0

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 3 is a protein called Monoclonal Antibody RVA122 Light Chain.

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

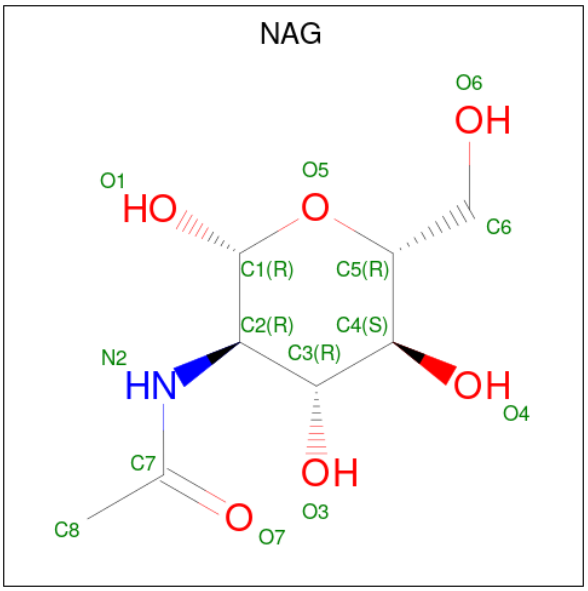
- Molecule 4 is a protein called Monoclonal Antibody 8C5 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	109	831	519	147	162	3	0	0
4	L	109	831	519	147	162	3	0	0
4	N	109	831	519	147	162	3	0	0

- Molecule 5 is a protein called Monoclonal Antibody 8C5 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	119	922	587	156	175	4	0	0
5	M	119	922	587	156	175	4	0	0
5	o	119	922	587	156	175	4	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



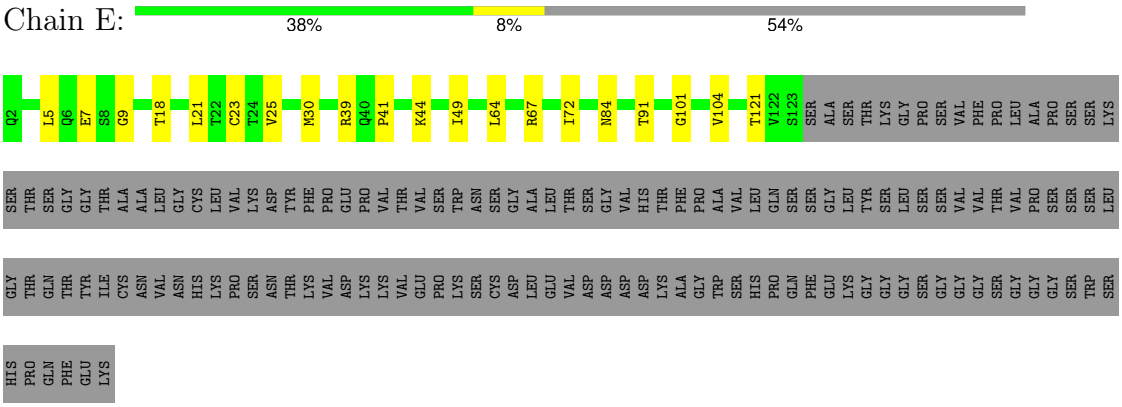
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	C	1	14	8	1	5	0
6	C	1	14	8	1	5	0
6	C	1	14	8	1	5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

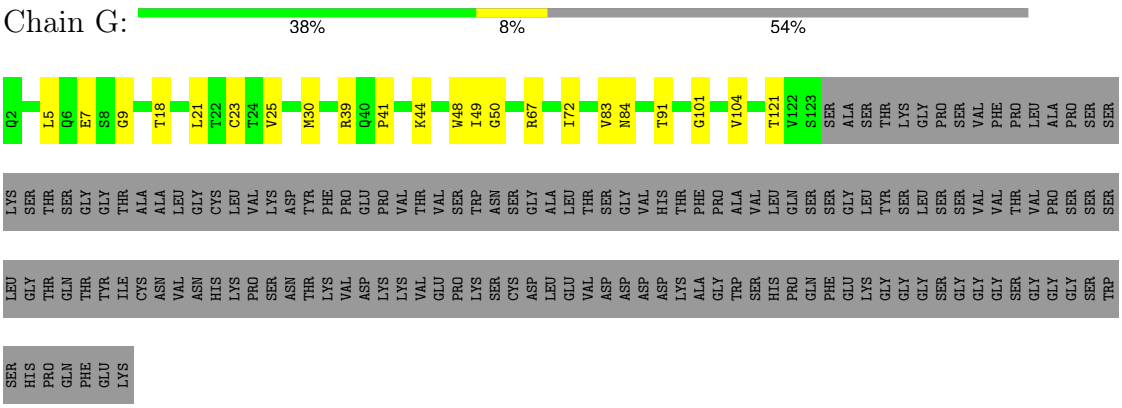
• Molecule 1: Monoclonal Antibody RVA122 Heavy Chain

Chain E:



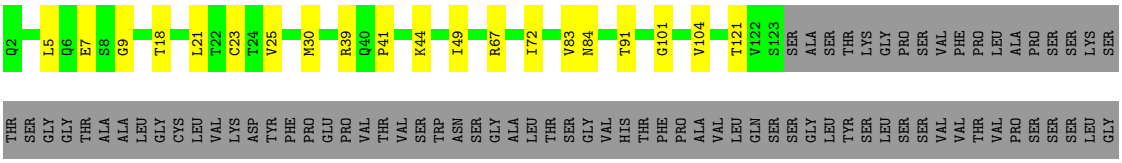
• Molecule 1: Monoclonal Antibody RVA122 Heavy Chain

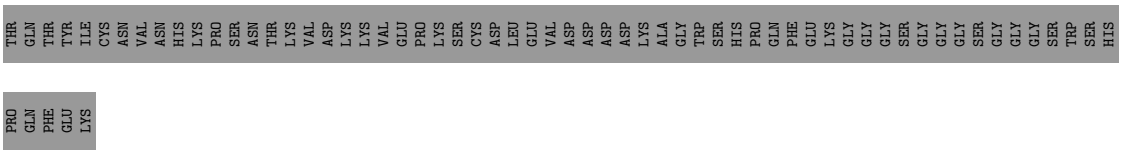
Chain G:



• Molecule 1: Monoclonal Antibody RVA122 Heavy Chain

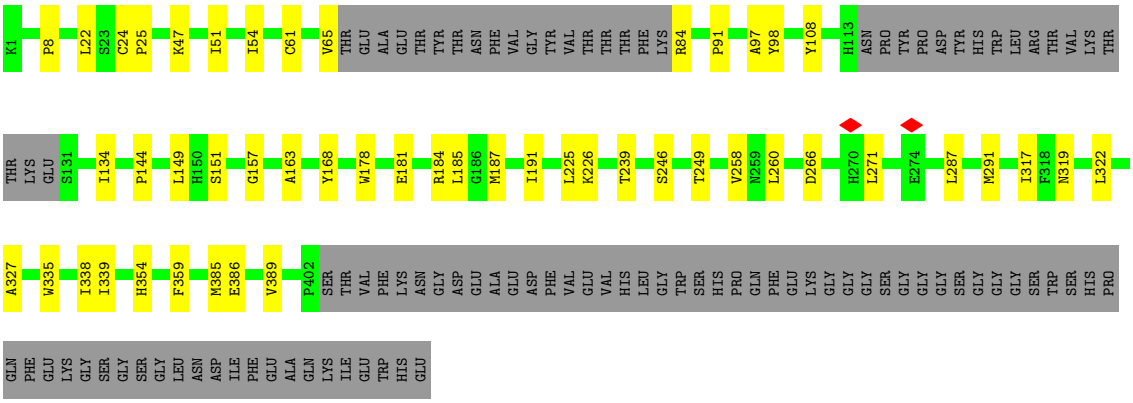
Chain I:





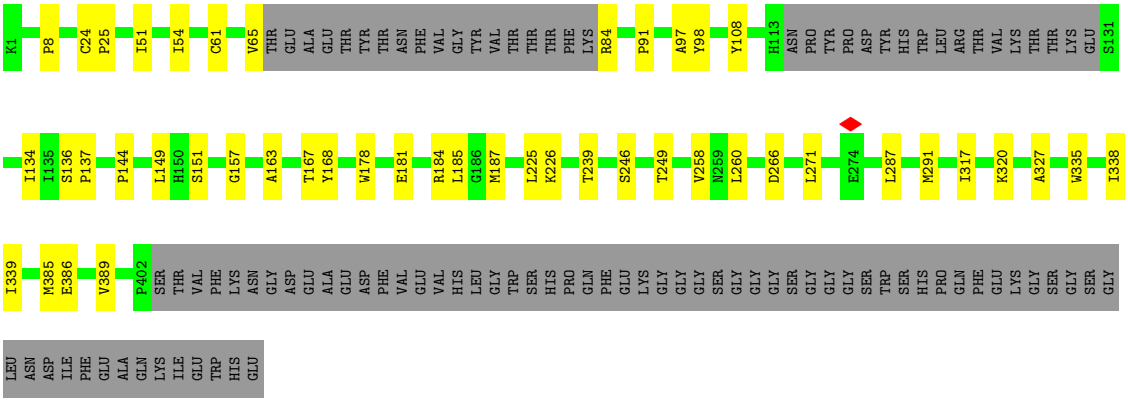
- Molecule 2: Glycoprotein

Chain A:



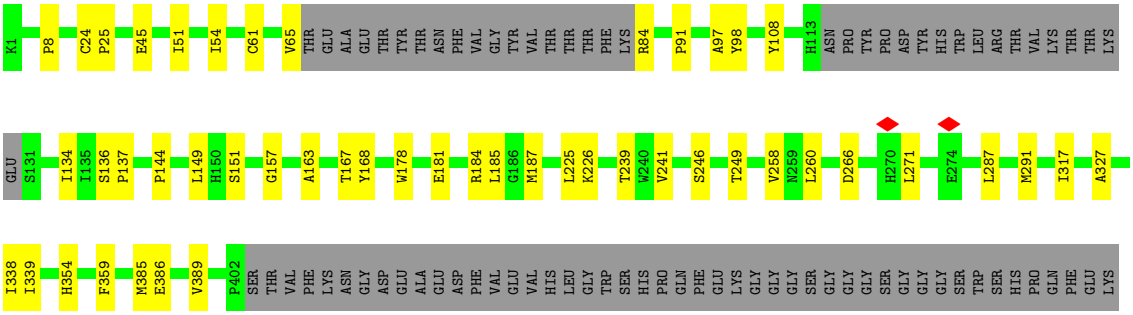
- Molecule 2: Glycoprotein

Chain B:



- Molecule 2: Glycoprotein

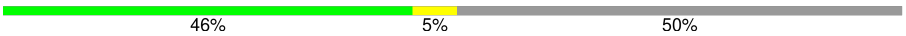
Chain C:



GLY SER GLY SER GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU

- Molecule 3: Monoclonal Antibody RVA122 Light Chain

Chain H:



GLN S2 R17 V18 T19 I29 V34 Y35 W36 I49 A75 I76 S77 E84 L107 L110 GLY THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU

ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU ARG SER

PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

- Molecule 3: Monoclonal Antibody RVA122 Light Chain

Chain D:

GLN S2 R17 V18 T19 I29 V34 Y35 W36 I49 A75 E84 L107 L110 GLY THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS

VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU ARG SER PRO VAL

THR LYS SER PHE ASN ARG GLY GLU CYS

- Molecule 3: Monoclonal Antibody RVA122 Light Chain

Chain F:

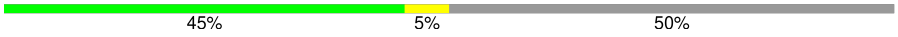
GLN S2 R17 V18 T19 I29 V34 Y35 W36 I49 A75 E84 L107 L110 GLY THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS

VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU ARG SER PRO VAL

THR LYS SER PHE ASN ARG GLY GLU CYS

- Molecule 4: Monoclonal Antibody 8C5 Light Chain

Chain J:



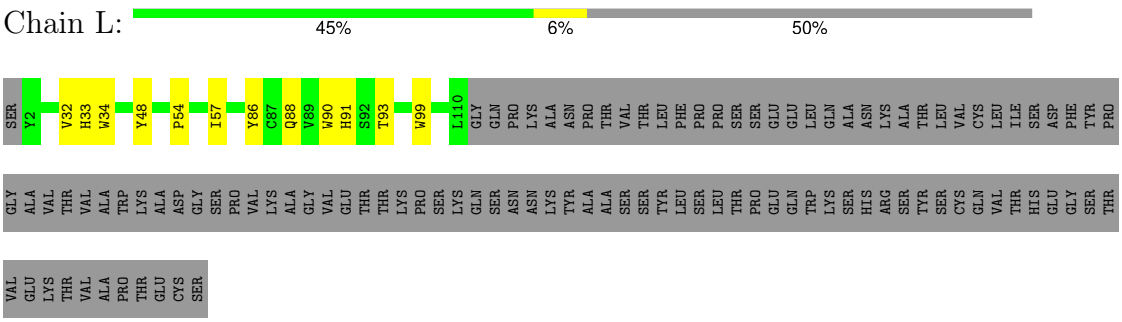
SER Y2 V32 H33 W34 Y48 P54 Y86 C87 Q88 V89 W90 H91 S92 T93 W99 L110 GLY GLN PRO LYS ALA ASN PRO THR VAL THR LEU PHE PRO PRO SER SER GLU GLU LEU GLN ALA ASN LYS ALA THR LEU VAL CYS LEU ILE SER ASP PHE TYR PRO GLY ALA

VAL THR VAL ALA TRP LYS ALA ASP GLY SER PRO VAL LYS ALA GLY VAL GLU THR THR LYS PRO SER LYS GLN SER ASN ASN LYS TYR ALA ALA SER SER TYR LEU SER LEU THR PRO GLU GLN TRP LYS SER HIS ARG SER TYR SER CYS GLN VAL THR HIS GLU GLY SER THR VAL GLU

LYS THR VAL ALA PRO THR GLU CYS SER

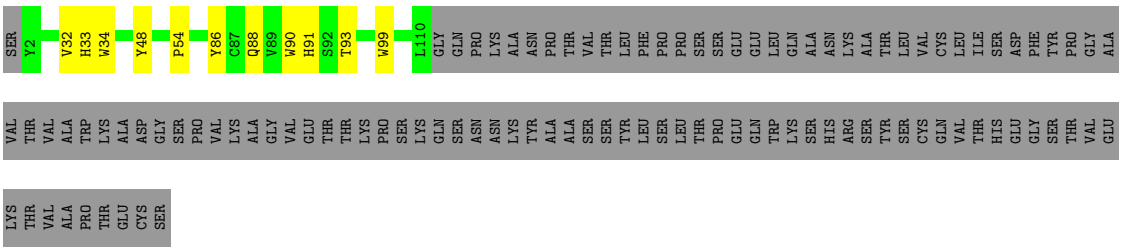
- Molecule 4: Monoclonal Antibody 8C5 Light Chain

Chain L:



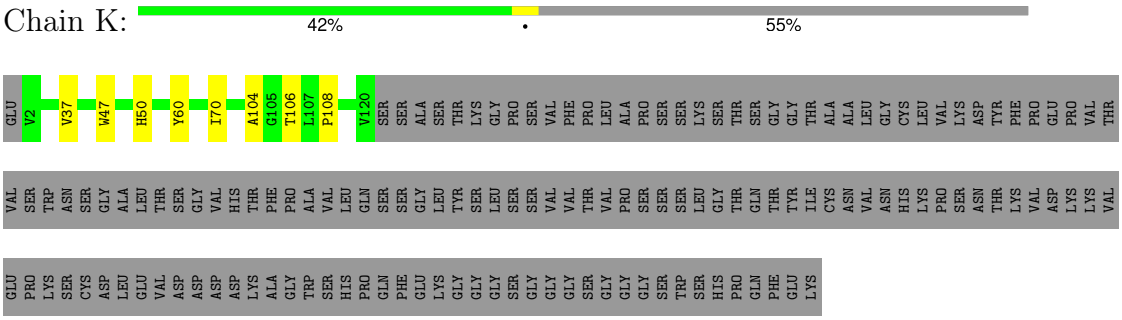
- Molecule 4: Monoclonal Antibody 8C5 Light Chain

Chain N:



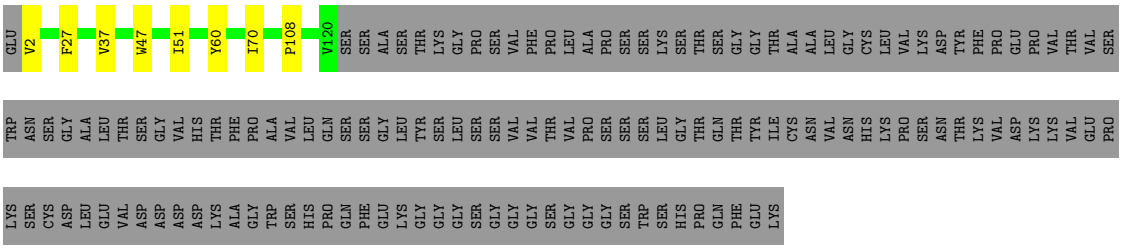
- Molecule 5: Monoclonal Antibody 8C5 Heavy Chain

Chain K:



- Molecule 5: Monoclonal Antibody 8C5 Heavy Chain

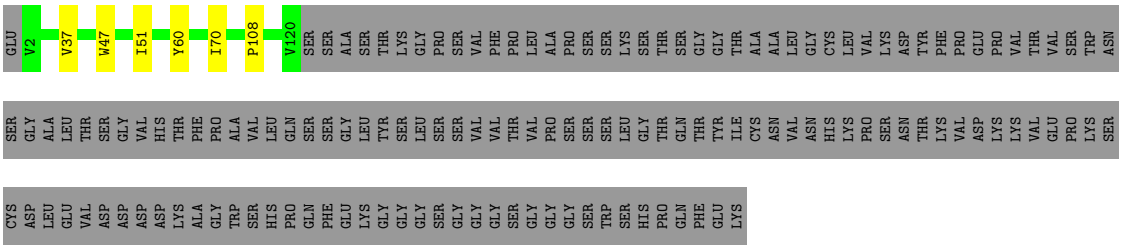
Chain M:



- Molecule 5: Monoclonal Antibody 8C5 Heavy Chain

Chain o:

43%
55%


GLU V2 V37 W47 I51 Y60 I70 P108 V120 SER SER ALA SER THR LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN
SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER
CYS ASP LEU GLU VAL ASP ASP ASP ASP LYS ALA GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208987	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	0.592	Depositor
Minimum map value	-0.160	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	E	0.20	0/979	0.35	0/1338
1	G	0.20	0/979	0.35	0/1338
1	I	0.20	0/979	0.35	0/1338
2	A	0.23	0/2936	0.38	0/3975
2	B	0.23	0/2936	0.36	0/3975
2	C	0.22	0/2936	0.37	0/3975
3	D	0.19	0/836	0.32	0/1137
3	F	0.19	0/836	0.32	0/1137
3	H	0.19	0/836	0.32	0/1137
4	J	0.20	0/853	0.38	0/1163
4	L	0.20	0/853	0.38	0/1163
4	N	0.20	0/853	0.38	0/1163
5	K	0.17	0/948	0.38	0/1289
5	M	0.17	0/948	0.37	0/1289
5	o	0.17	0/948	0.37	0/1289
All	All	0.21	0/19656	0.36	0/26706

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	E	0	1
1	G	0	1
1	I	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	67	ARG	Sidechain
1	G	67	ARG	Sidechain
1	I	67	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	E	952	0	898	10	0
1	G	952	0	898	11	0
1	I	952	0	898	10	0
2	A	2866	0	2831	31	0
2	B	2866	0	2831	29	0
2	C	2866	0	2831	28	0
3	D	816	0	778	6	0
3	F	816	0	778	6	0
3	H	816	0	778	7	0
4	J	831	0	789	10	0
4	L	831	0	789	10	0
4	N	831	0	789	9	0
5	K	922	0	865	5	0
5	M	922	0	865	5	0
5	o	922	0	865	4	0
6	A	42	0	39	2	0
6	B	42	0	39	2	0
6	C	42	0	39	0	0
All	All	19287	0	18600	174	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 5.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LYS:HZ2	6:B:503:NAG:H82	1.64	0.62
2:C:98:TYR:OH	2:C:181:GLU:HG2	2.01	0.61
2:A:98:TYR:OH	2:A:181:GLU:HG2	2.01	0.60
2:B:98:TYR:OH	2:B:181:GLU:HG2	2.01	0.60
2:C:287:LEU:HD11	2:C:291:MET:HE2	1.85	0.59
2:C:61:CYS:HA	2:C:134:ILE:HG22	1.85	0.59
2:B:61:CYS:HA	2:B:134:ILE:HG22	1.86	0.58
2:B:287:LEU:HD11	2:B:291:MET:HE2	1.85	0.58
4:J:90:TRP:CD2	4:J:91:HIS:HB3	2.40	0.57
1:E:5:LEU:HD22	1:E:25:VAL:HG22	1.87	0.57
2:A:61:CYS:HA	2:A:134:ILE:HG22	1.86	0.57
4:L:90:TRP:CD2	4:L:91:HIS:HB3	2.40	0.57
2:C:51:ILE:HD11	2:C:239:THR:HA	1.86	0.56
1:G:5:LEU:HD22	1:G:25:VAL:HG22	1.85	0.56
1:I:5:LEU:HD22	1:I:25:VAL:HG22	1.87	0.56
4:N:90:TRP:CD2	4:N:91:HIS:HB3	2.40	0.56
2:A:266:ASP:HB3	2:A:271:LEU:HD11	1.88	0.56
2:B:266:ASP:HB3	2:B:271:LEU:HD11	1.88	0.56
2:A:287:LEU:HD11	2:A:291:MET:HE2	1.86	0.55
2:B:97:ALA:HB1	2:B:108:TYR:HE1	1.72	0.55
2:C:97:ALA:HB1	2:C:108:TYR:HE1	1.72	0.55
5:K:37:VAL:HG12	5:K:47:TRP:HA	1.89	0.55
2:C:266:ASP:HB3	2:C:271:LEU:HD11	1.89	0.54
2:C:338:ILE:HG13	2:C:339:ILE:HD12	1.90	0.54
2:B:338:ILE:HG13	2:B:339:ILE:HD12	1.90	0.53
5:M:37:VAL:HG12	5:M:47:TRP:HA	1.90	0.53
2:A:97:ALA:HB1	2:A:108:TYR:HE1	1.72	0.53
5:o:37:VAL:HG12	5:o:47:TRP:HA	1.89	0.53
2:A:338:ILE:HG13	2:A:339:ILE:HD12	1.91	0.53
3:F:36:TRP:HD1	3:F:49:ILE:HD11	1.73	0.53
4:J:33:HIS:CD2	5:K:108:PRO:HB3	2.44	0.53
3:H:36:TRP:HD1	3:H:49:ILE:HD11	1.74	0.53
2:B:320:LYS:NZ	6:B:503:NAG:H82	2.23	0.53
3:F:36:TRP:CD1	3:F:49:ILE:HD11	2.44	0.52
4:N:33:HIS:CD2	5:o:108:PRO:HB3	2.44	0.52
3:H:36:TRP:CD1	3:H:49:ILE:HD11	2.45	0.51
2:C:91:PRO:HD3	2:C:168:TYR:CE1	2.46	0.51
1:G:7:GLU:HG3	1:G:23:CYS:HB3	1.92	0.51
2:B:91:PRO:HD3	2:B:168:TYR:CE1	2.46	0.51
2:A:91:PRO:HD3	2:A:168:TYR:CE1	2.46	0.51
3:D:36:TRP:CD1	3:D:49:ILE:HD11	2.45	0.51
3:D:36:TRP:HD1	3:D:49:ILE:HD11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ILE:HG21	2:B:187:MET:HE1	1.93	0.51
1:G:91:THR:HG23	1:G:121:THR:HA	1.93	0.50
2:C:317:ILE:O	2:C:317:ILE:HG22	2.11	0.50
3:F:19:THR:HG22	3:F:75:ALA:HB2	1.93	0.50
4:L:33:HIS:CD2	5:M:108:PRO:HB3	2.47	0.50
2:A:246:SER:HB3	2:A:249:THR:HG23	1.94	0.50
1:E:7:GLU:HG3	1:E:23:CYS:HB3	1.94	0.49
3:D:19:THR:HG22	3:D:75:ALA:HB2	1.93	0.49
1:E:91:THR:HG23	1:E:121:THR:HA	1.93	0.49
2:C:246:SER:HB3	2:C:249:THR:HG23	1.94	0.49
1:I:18:THR:HG22	1:I:84:ASN:HA	1.94	0.49
2:B:51:ILE:HD11	2:B:239:THR:HA	1.95	0.49
2:A:317:ILE:HG22	2:A:317:ILE:O	2.11	0.49
3:H:19:THR:HG22	3:H:75:ALA:HB2	1.93	0.49
1:G:30:MET:HE1	1:G:72:ILE:HD11	1.95	0.48
1:E:18:THR:HG22	1:E:84:ASN:HA	1.95	0.48
1:I:7:GLU:HG3	1:I:23:CYS:HB3	1.95	0.48
1:I:30:MET:HE1	1:I:72:ILE:HD11	1.95	0.48
1:I:91:THR:HG23	1:I:121:THR:HA	1.95	0.48
4:L:48:TYR:HD1	4:L:54:PRO:HD3	1.79	0.48
3:D:29:ILE:HD12	3:D:34:VAL:HG22	1.96	0.48
4:N:48:TYR:HD1	4:N:54:PRO:HD3	1.79	0.47
2:B:246:SER:HB3	2:B:249:THR:HG23	1.96	0.47
4:N:90:TRP:HD1	4:N:99:TRP:CE2	2.32	0.47
2:A:51:ILE:HD11	2:A:239:THR:HA	1.96	0.47
2:A:335:TRP:HE3	2:A:338:ILE:HD11	1.80	0.47
4:J:48:TYR:HD1	4:J:54:PRO:HD3	1.80	0.47
2:A:54:ILE:HG21	2:A:187:MET:HE1	1.97	0.47
2:A:65:VAL:O	2:A:84:ARG:HD3	2.15	0.47
2:B:65:VAL:O	2:B:84:ARG:HD3	2.15	0.47
2:A:8:PRO:HB3	2:A:327:ALA:HB1	1.97	0.47
5:M:60:TYR:CE1	5:M:70:ILE:HG22	2.51	0.46
2:C:54:ILE:HG21	2:C:187:MET:HE1	1.96	0.46
1:E:39:ARG:HB2	1:E:49:ILE:HD11	1.96	0.46
1:G:41:PRO:HB2	1:G:44:LYS:HD2	1.98	0.46
2:C:8:PRO:HB3	2:C:327:ALA:HB1	1.97	0.46
3:F:29:ILE:HD12	3:F:34:VAL:HG22	1.98	0.46
2:C:24:CYS:SG	2:C:25:PRO:HD2	2.56	0.46
2:C:65:VAL:O	2:C:84:ARG:HD3	2.15	0.46
5:K:60:TYR:CE1	5:K:70:ILE:HG22	2.51	0.46
4:J:32:VAL:HA	4:J:88:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ILE:HG22	2:B:317:ILE:O	2.16	0.45
2:A:24:CYS:SG	2:A:25:PRO:HD2	2.56	0.45
4:J:91:HIS:HD2	4:J:93:THR:C	2.23	0.45
2:C:225:LEU:HD23	2:C:226:LYS:N	2.32	0.45
1:G:101:GLY:O	1:G:104:VAL:HG12	2.17	0.45
2:B:335:TRP:HE3	2:B:338:ILE:HD11	1.82	0.45
1:I:101:GLY:O	1:I:104:VAL:HG12	2.17	0.45
2:B:24:CYS:SG	2:B:25:PRO:HD2	2.57	0.45
5:K:50:HIS:NE2	5:K:104:ALA:HB2	2.32	0.45
5:o:60:TYR:CE1	5:o:70:ILE:HG22	2.51	0.45
2:A:319:ASN:OD1	6:A:503:NAG:N2	2.50	0.45
4:J:34:TRP:HA	4:J:86:TYR:O	2.17	0.45
4:J:90:TRP:HD1	4:J:99:TRP:CE2	2.35	0.45
1:I:39:ARG:HB2	1:I:49:ILE:HD11	1.99	0.45
1:G:18:THR:HG22	1:G:84:ASN:HA	1.98	0.44
1:E:30:MET:HE1	1:E:72:ILE:HD11	1.98	0.44
1:G:39:ARG:HB2	1:G:49:ILE:HD11	2.00	0.44
2:A:22:LEU:HD21	2:A:322:LEU:HD21	2.00	0.44
4:L:90:TRP:HD1	4:L:99:TRP:CE2	2.34	0.44
4:L:91:HIS:HD2	4:L:93:THR:C	2.24	0.44
2:C:386:GLU:O	2:C:389:VAL:HG12	2.17	0.44
1:I:41:PRO:HB2	1:I:44:LYS:HD2	1.98	0.44
2:B:225:LEU:HD23	2:B:226:LYS:N	2.33	0.44
2:B:54:ILE:HD13	2:B:144:PRO:HD3	2.00	0.44
2:A:151:SER:O	2:A:157:GLY:HA2	2.18	0.44
2:A:354:HIS:HB3	2:A:359:PHE:CE1	2.53	0.44
3:H:29:ILE:HD12	3:H:34:VAL:HG22	1.99	0.43
1:E:101:GLY:O	1:E:104:VAL:HG12	2.17	0.43
2:A:225:LEU:HD23	2:A:226:LYS:N	2.33	0.43
4:N:91:HIS:HD2	4:N:93:THR:C	2.26	0.43
1:I:9:GLY:HA3	1:I:21:LEU:HD23	2.00	0.43
4:N:34:TRP:HA	4:N:86:TYR:O	2.18	0.43
4:L:32:VAL:HA	4:L:88:GLN:O	2.18	0.43
4:L:90:TRP:CD1	4:L:99:TRP:CE2	3.07	0.43
2:A:385:MET:HE1	2:C:291:MET:SD	2.59	0.43
4:L:34:TRP:HA	4:L:86:TYR:O	2.19	0.43
2:B:386:GLU:O	2:B:389:VAL:HG12	2.18	0.43
2:B:184:ARG:NH2	2:B:185:LEU:HB2	2.34	0.42
1:E:41:PRO:HB2	1:E:44:LYS:HD2	2.00	0.42
4:J:90:TRP:CE3	5:K:106:THR:HG22	2.53	0.42
2:C:54:ILE:HD13	2:C:144:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:151:SER:O	2:C:157:GLY:HA2	2.19	0.42
4:N:32:VAL:HA	4:N:88:GLN:O	2.18	0.42
2:A:184:ARG:NH2	2:A:185:LEU:HB2	2.34	0.42
2:C:184:ARG:NH2	2:C:185:LEU:HB2	2.34	0.42
2:A:386:GLU:O	2:A:389:VAL:HG12	2.19	0.42
3:F:17:ARG:HH21	3:F:75:ALA:HB1	1.85	0.42
2:A:291:MET:SD	2:B:385:MET:HE1	2.60	0.42
2:A:47:LYS:HZ2	2:A:191:ILE:C	2.28	0.42
3:H:84:GLU:HB2	3:H:107:LEU:O	2.20	0.42
4:N:90:TRP:CD1	4:N:99:TRP:CE2	3.08	0.42
2:B:151:SER:O	2:B:157:GLY:HA2	2.19	0.42
2:C:45:GLU:HB3	2:C:241:VAL:HG12	2.02	0.42
2:A:163:ALA:HB2	2:A:185:LEU:HD12	2.02	0.42
2:A:258:VAL:HG13	2:A:260:LEU:HD22	2.02	0.42
2:B:291:MET:SD	2:C:385:MET:HE1	2.60	0.42
2:A:54:ILE:HD13	2:A:144:PRO:HD3	2.03	0.41
2:A:317:ILE:HD13	2:A:317:ILE:HG21	1.89	0.41
3:D:17:ARG:HH21	3:D:75:ALA:HB1	1.85	0.41
2:B:163:ALA:HB2	2:B:185:LEU:HD12	2.02	0.41
3:F:84:GLU:HB2	3:F:107:LEU:O	2.20	0.41
2:B:8:PRO:HB3	2:B:327:ALA:HB1	2.03	0.41
2:C:354:HIS:HB3	2:C:359:PHE:CE1	2.55	0.41
5:M:51:ILE:HD12	5:M:51:ILE:HA	1.91	0.41
2:A:149:LEU:HD22	2:A:178:TRP:CH2	2.56	0.41
4:L:48:TYR:CD1	4:L:54:PRO:HD3	2.55	0.41
3:H:17:ARG:HH21	3:H:75:ALA:HB1	1.85	0.41
2:C:149:LEU:HD22	2:C:178:TRP:CH2	2.55	0.41
1:G:48:TRP:CZ2	1:G:50:GLY:HA2	2.56	0.41
2:C:163:ALA:HB2	2:C:185:LEU:HD12	2.02	0.41
1:G:9:GLY:HA3	1:G:21:LEU:HD23	2.03	0.41
1:G:18:THR:HA	1:G:83:VAL:O	2.20	0.41
3:D:84:GLU:HB2	3:D:107:LEU:O	2.20	0.41
4:L:57:ILE:HD13	4:L:57:ILE:HA	1.88	0.41
4:N:48:TYR:CD1	4:N:54:PRO:HD3	2.55	0.41
5:M:2:VAL:HG11	5:M:27:PHE:HB3	2.02	0.41
5:o:51:ILE:HD12	5:o:51:ILE:HA	1.90	0.41
3:H:17:ARG:CD	3:H:77:SER:HA	2.51	0.41
4:J:48:TYR:CD1	4:J:54:PRO:HD3	2.56	0.41
1:I:18:THR:HA	1:I:83:VAL:O	2.20	0.41
2:B:149:LEU:HD22	2:B:178:TRP:CH2	2.56	0.41
2:C:136:SER:N	2:C:137:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:THR:HG21	2:B:178:TRP:CZ3	2.56	0.40
2:C:167:THR:HG21	2:C:178:TRP:CZ3	2.56	0.40
1:E:9:GLY:HA3	1:E:21:LEU:HD23	2.02	0.40
2:A:319:ASN:OD1	6:A:503:NAG:C7	2.70	0.40
4:J:90:TRP:CD1	4:J:99:TRP:CE2	3.09	0.40
2:B:258:VAL:HG13	2:B:260:LEU:HD22	2.02	0.40
1:E:39:ARG:NH2	1:E:64:LEU:HD11	2.37	0.40
2:B:136:SER:N	2:B:137:PRO:CD	2.84	0.40
2:C:258:VAL:HG13	2:C:260:LEU:HD22	2.02	0.40

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	E	120/265 (45%)	117 (98%)	3 (2%)	0	100	100
1	G	120/265 (45%)	117 (98%)	3 (2%)	0	100	100
1	I	120/265 (45%)	117 (98%)	3 (2%)	0	100	100
2	A	361/468 (77%)	350 (97%)	11 (3%)	0	100	100
2	B	361/468 (77%)	349 (97%)	12 (3%)	0	100	100
2	C	361/468 (77%)	347 (96%)	14 (4%)	0	100	100
3	D	107/217 (49%)	105 (98%)	2 (2%)	0	100	100
3	F	107/217 (49%)	105 (98%)	2 (2%)	0	100	100
3	H	107/217 (49%)	106 (99%)	1 (1%)	0	100	100
4	J	107/216 (50%)	103 (96%)	4 (4%)	0	100	100
4	L	107/216 (50%)	103 (96%)	4 (4%)	0	100	100
4	N	107/216 (50%)	103 (96%)	4 (4%)	0	100	100
5	K	117/264 (44%)	114 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	117/264 (44%)	114 (97%)	3 (3%)	0	100	100
5	o	117/264 (44%)	113 (97%)	4 (3%)	0	100	100
All	All	2436/4290 (57%)	2363 (97%)	73 (3%)	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	E	105/223 (47%)	105 (100%)	0	100	100
1	G	105/223 (47%)	105 (100%)	0	100	100
1	I	105/223 (47%)	105 (100%)	0	100	100
2	A	323/406 (80%)	323 (100%)	0	100	100
2	B	323/406 (80%)	323 (100%)	0	100	100
2	C	323/406 (80%)	323 (100%)	0	100	100
3	D	90/186 (48%)	90 (100%)	0	100	100
3	F	90/186 (48%)	90 (100%)	0	100	100
3	H	90/186 (48%)	90 (100%)	0	100	100
4	J	89/181 (49%)	89 (100%)	0	100	100
4	L	89/181 (49%)	89 (100%)	0	100	100
4	N	89/181 (49%)	89 (100%)	0	100	100
5	K	96/216 (44%)	96 (100%)	0	100	100
5	M	96/216 (44%)	96 (100%)	0	100	100
5	o	96/216 (44%)	96 (100%)	0	100	100
All	All	2109/3636 (58%)	2109 (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. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	6	GLN
1	E	31	ASN
1	E	32	ASN
1	E	40	GLN
2	A	86	HIS
2	A	194	ASN
2	A	259	ASN
3	H	39	GLN
4	J	37	GLN
1	G	6	GLN
1	G	31	ASN
1	G	32	ASN
1	G	40	GLN
1	I	6	GLN
1	I	31	ASN
1	I	32	ASN
1	I	40	GLN
3	D	39	GLN
3	F	39	GLN
4	L	37	GLN
4	N	26	ASN
4	N	37	GLN
2	B	27	ASN
2	B	86	HIS
2	B	99	ASN
2	C	27	ASN
2	C	86	HIS
5	K	39	GLN
5	K	50	HIS
5	K	114	GLN
5	M	39	GLN
5	M	114	GLN
5	o	35	HIS
5	o	39	GLN
5	o	50	HIS
5	o	114	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands 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	$\#\|Z\| > 2$
6	NAG	B	501	2	14,14,15	0.68	0	17,19,21	0.90	1 (5%)
6	NAG	C	503	2	14,14,15	0.60	0	17,19,21	1.34	1 (5%)
6	NAG	A	502	2	14,14,15	0.63	0	17,19,21	1.37	1 (5%)
6	NAG	A	501	2	14,14,15	0.68	0	17,19,21	0.89	1 (5%)
6	NAG	B	503	2	14,14,15	0.72	0	17,19,21	0.82	0
6	NAG	A	503	2	14,14,15	1.03	1 (7%)	17,19,21	1.16	1 (5%)
6	NAG	B	502	2	14,14,15	0.63	0	17,19,21	1.37	1 (5%)
6	NAG	C	501	2	14,14,15	0.68	0	17,19,21	0.89	1 (5%)
6	NAG	C	502	2	14,14,15	0.63	0	17,19,21	1.38	1 (5%)

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
6	NAG	B	501	2	-	2/6/23/26	0/1/1/1
6	NAG	C	503	2	-	2/6/23/26	0/1/1/1
6	NAG	A	502	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	501	2	-	2/6/23/26	0/1/1/1
6	NAG	B	503	2	-	0/6/23/26	0/1/1/1
6	NAG	A	503	2	-	0/6/23/26	0/1/1/1
6	NAG	B	502	2	-	2/6/23/26	0/1/1/1
6	NAG	C	501	2	-	2/6/23/26	0/1/1/1
6	NAG	C	502	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	503	NAG	C1-C2	3.14	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	502	NAG	C1-O5-C5	5.10	119.02	112.19
6	C	502	NAG	C1-O5-C5	5.09	119.01	112.19
6	A	502	NAG	C1-O5-C5	5.07	118.98	112.19
6	C	503	NAG	C1-O5-C5	4.94	118.80	112.19
6	A	503	NAG	C2-N2-C7	3.43	127.49	122.90
6	C	501	NAG	C1-O5-C5	2.44	115.45	112.19
6	A	501	NAG	C1-O5-C5	2.43	115.44	112.19
6	B	501	NAG	C1-O5-C5	2.42	115.43	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	NAG	C8-C7-N2-C2
6	A	501	NAG	O7-C7-N2-C2
6	B	501	NAG	C8-C7-N2-C2
6	B	501	NAG	O7-C7-N2-C2
6	C	501	NAG	C8-C7-N2-C2
6	C	501	NAG	O7-C7-N2-C2
6	A	502	NAG	O5-C5-C6-O6
6	C	502	NAG	O5-C5-C6-O6
6	B	502	NAG	O5-C5-C6-O6
6	C	503	NAG	C4-C5-C6-O6
6	C	503	NAG	O5-C5-C6-O6
6	C	502	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	502	NAG	C4-C5-C6-O6
6	B	502	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	503	NAG	2	0
6	A	503	NAG	2	0

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.

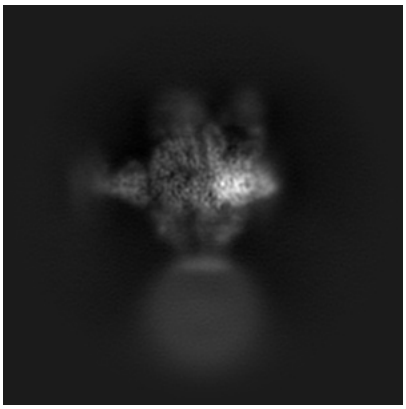
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-75814. These allow visual inspection of the internal detail of the map and identification of artifacts.

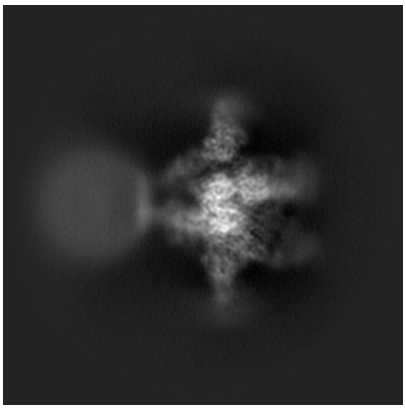
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

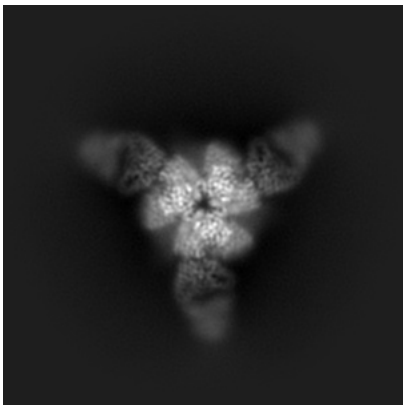
6.1.1 Primary map



X

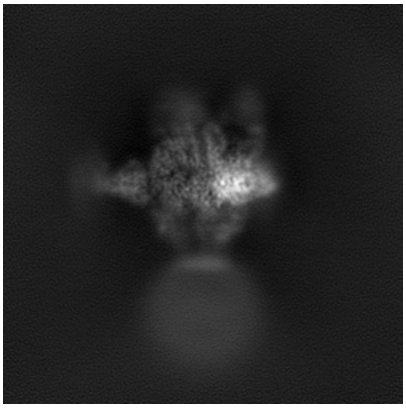


Y

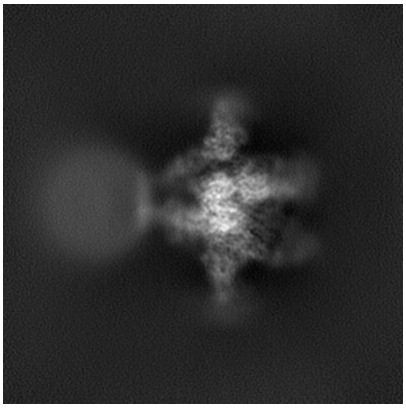


Z

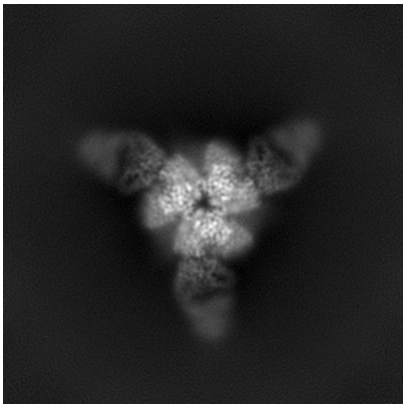
6.1.2 Raw map



X



Y

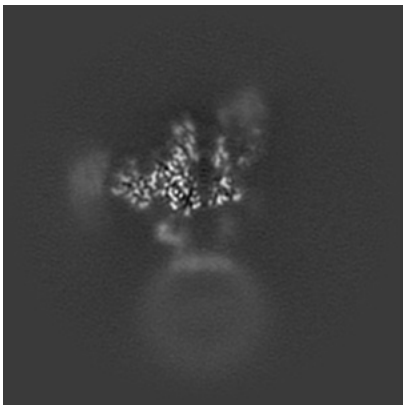


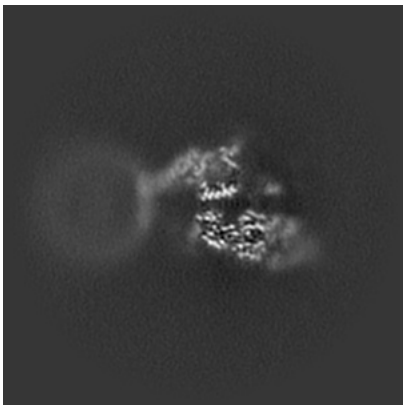
Z

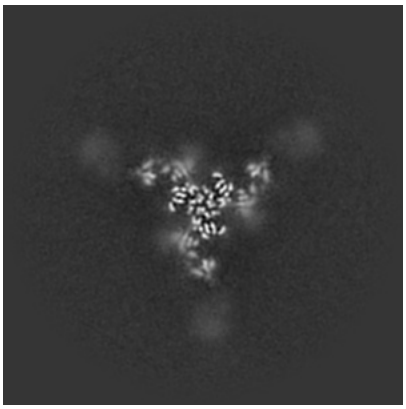
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

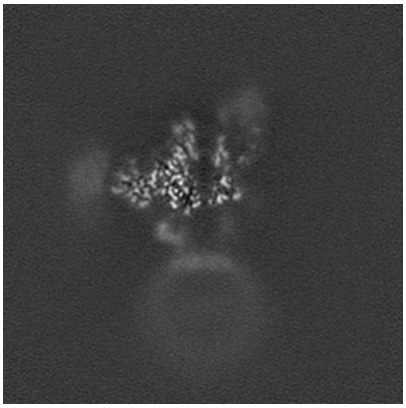
6.2.1 Primary map

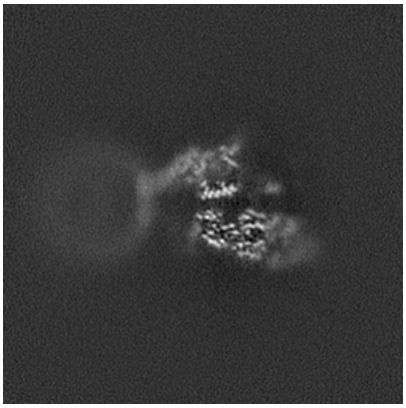

X Index: 128

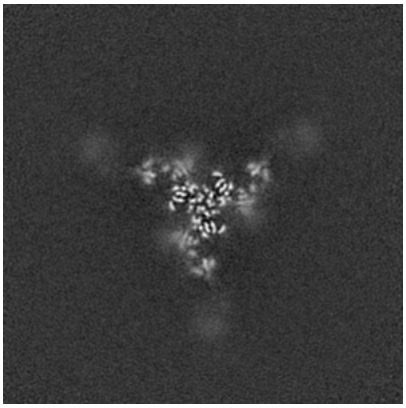

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

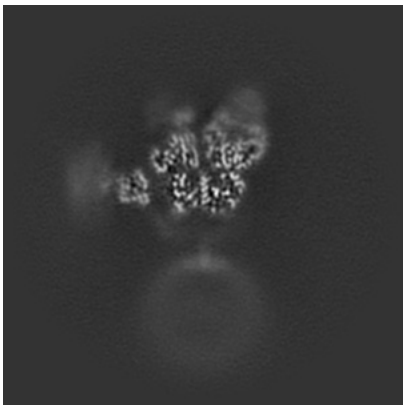

Y Index: 128

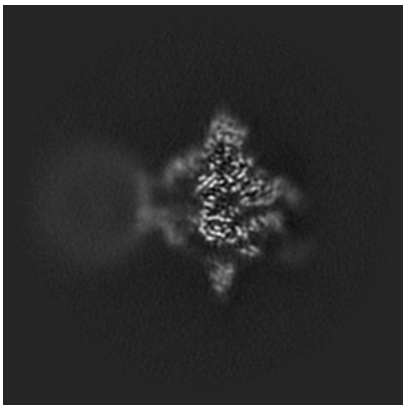

Z Index: 128

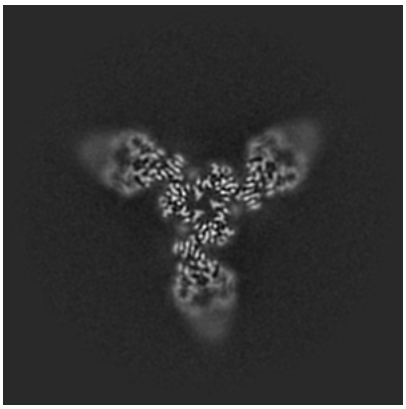
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

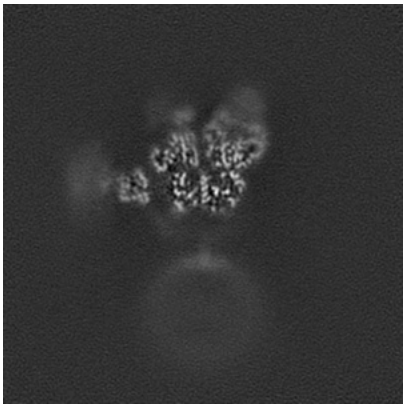
6.3.1 Primary map

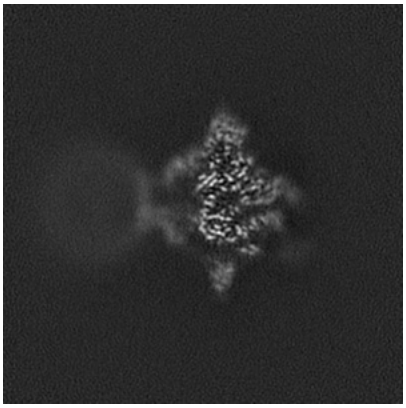

X Index: 135

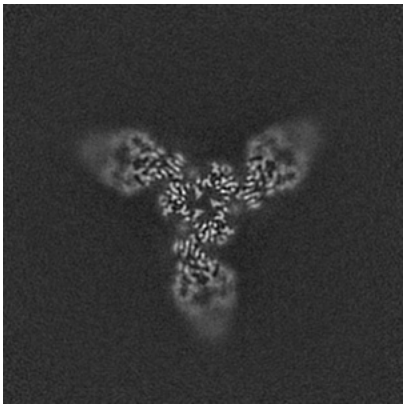

Y Index: 138


Z Index: 141

6.3.2 Raw map


X Index: 135

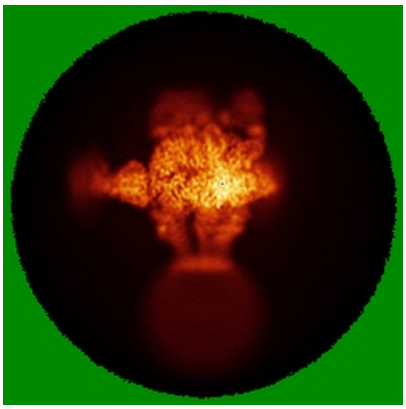

Y Index: 138

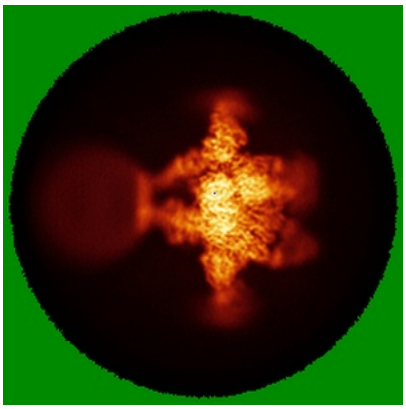

Z Index: 141

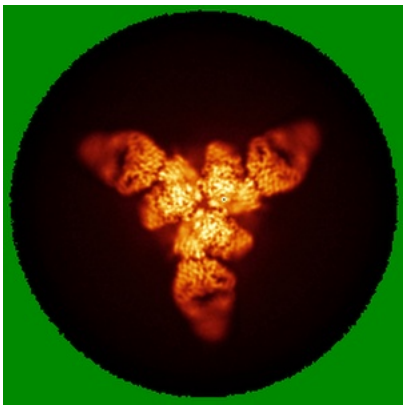
The images above show the largest variance slices of the map in three orthogonal directions.

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

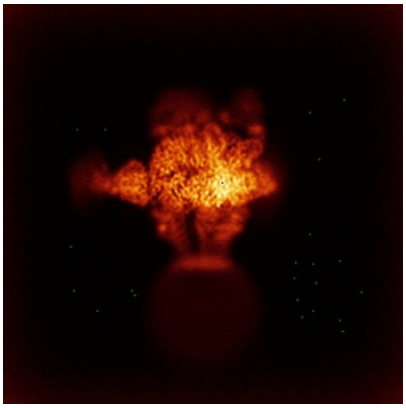
6.4.1 Primary map

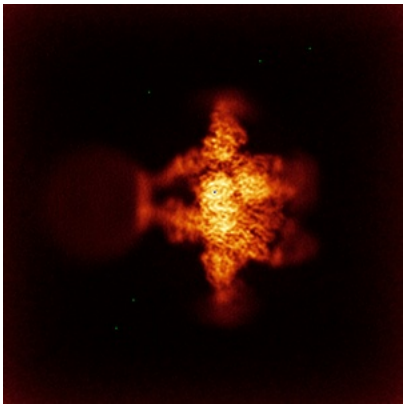

X

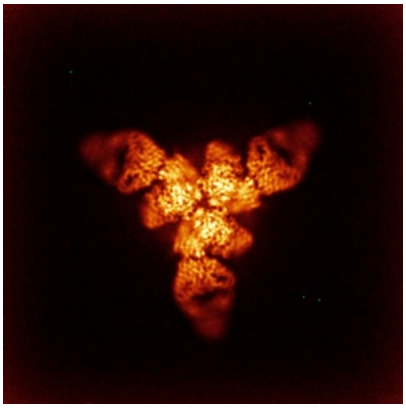

Y


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 0.1. 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.

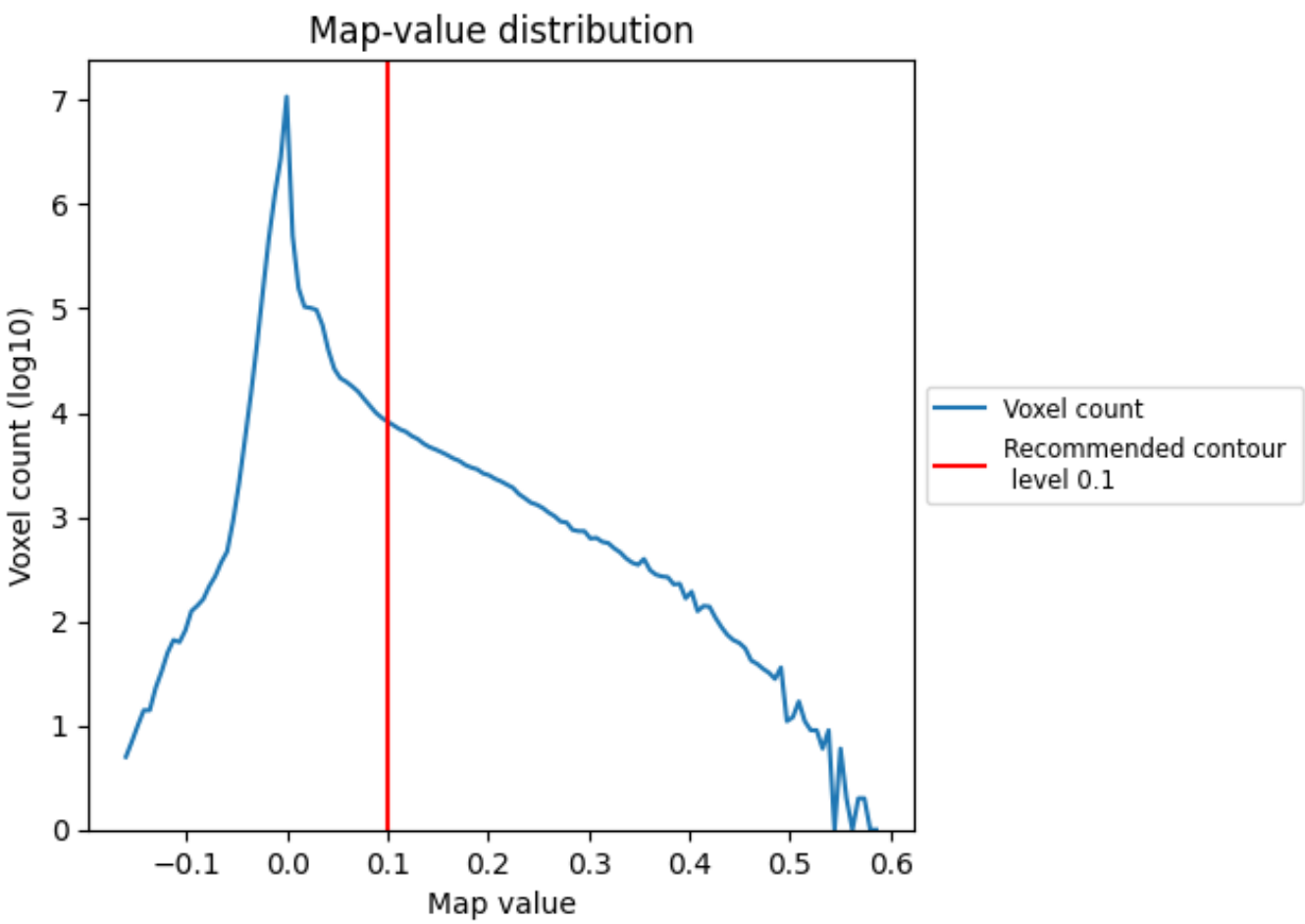
6.6 Mask visualisation (i)

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

7 Map analysis (i)

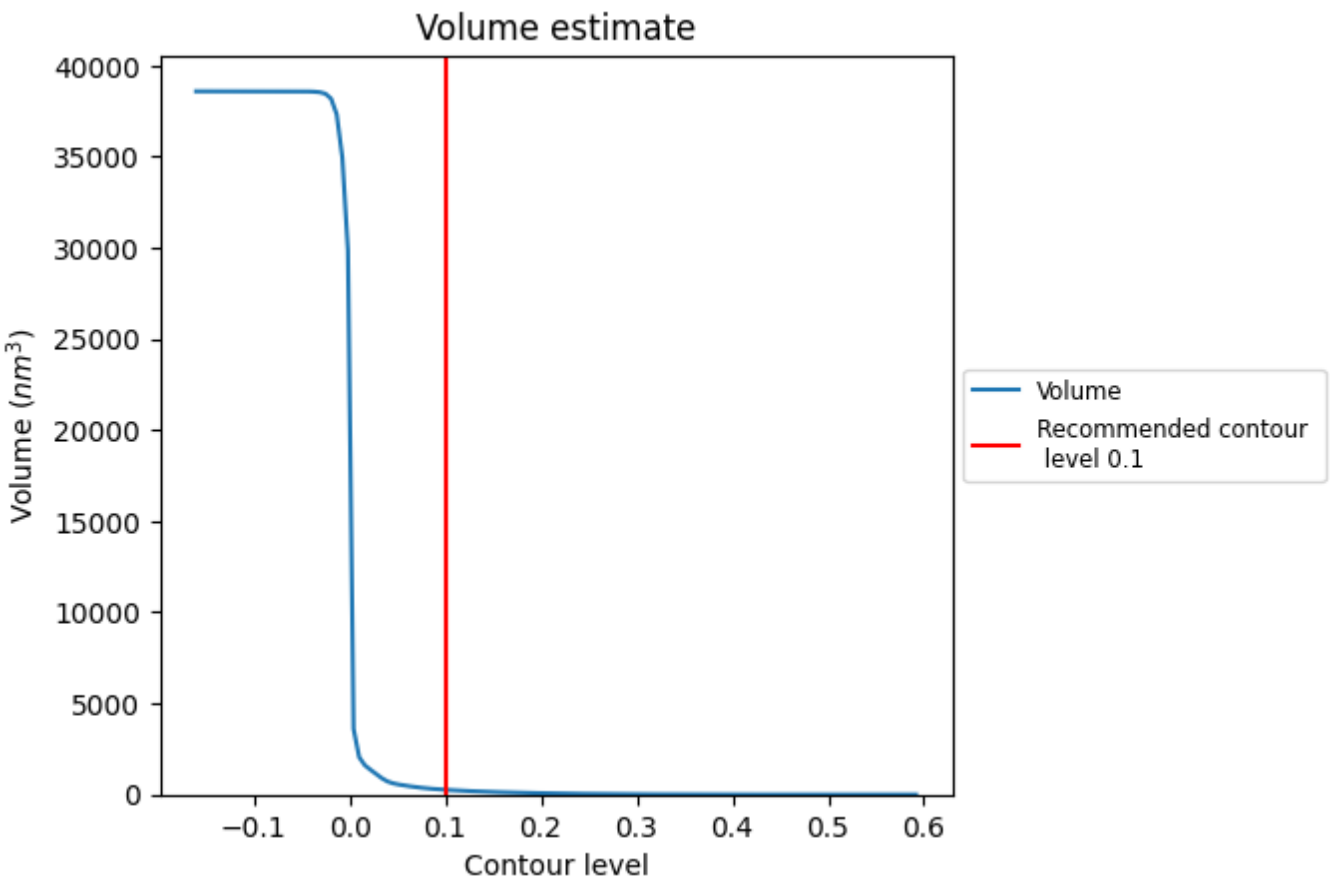
This section contains the results of statistical analysis of the map.

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.

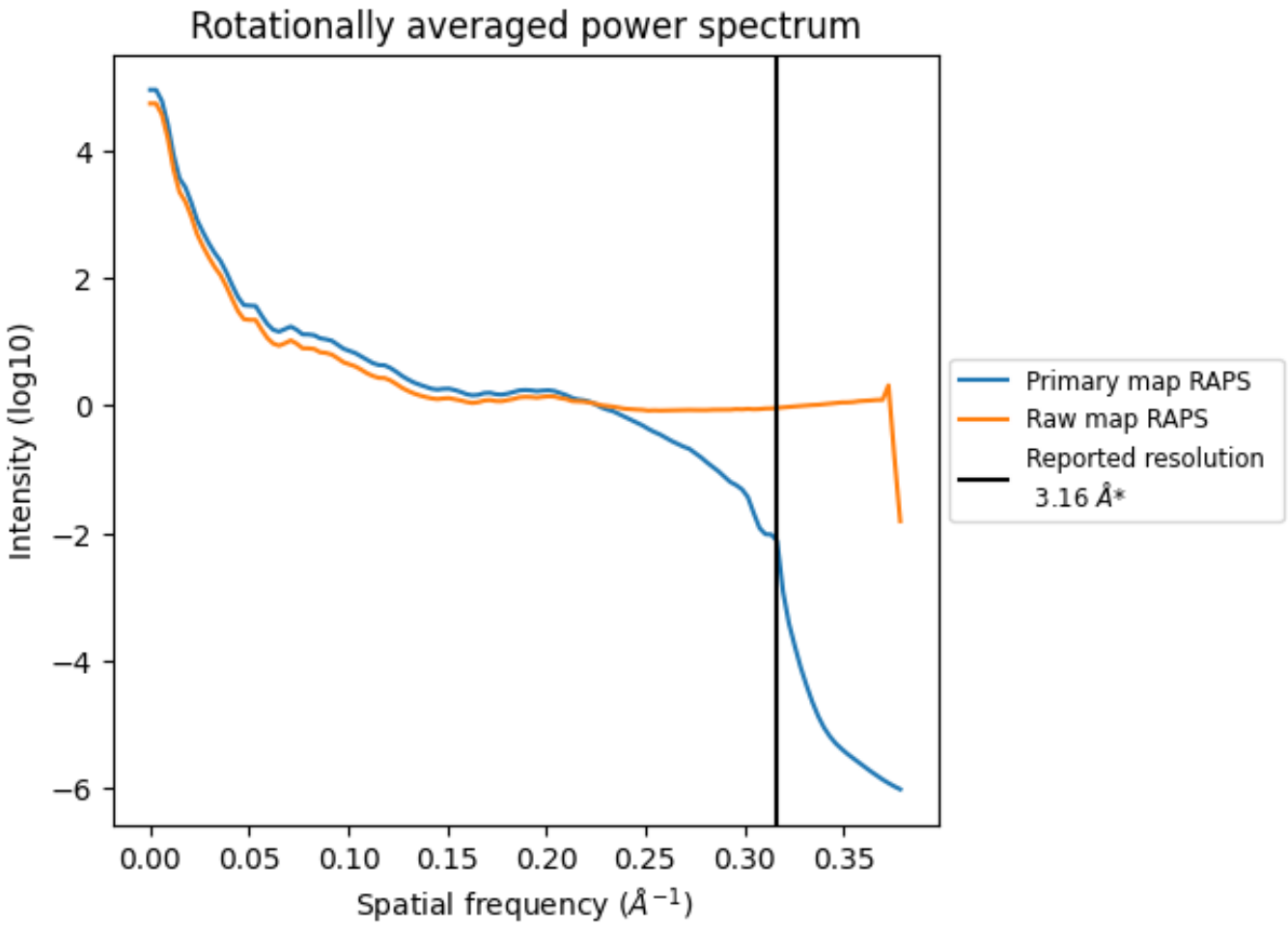
7.2 Volume estimate (i)



The volume at the recommended contour level is 264 nm^3; this corresponds to an approximate mass of 238 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)

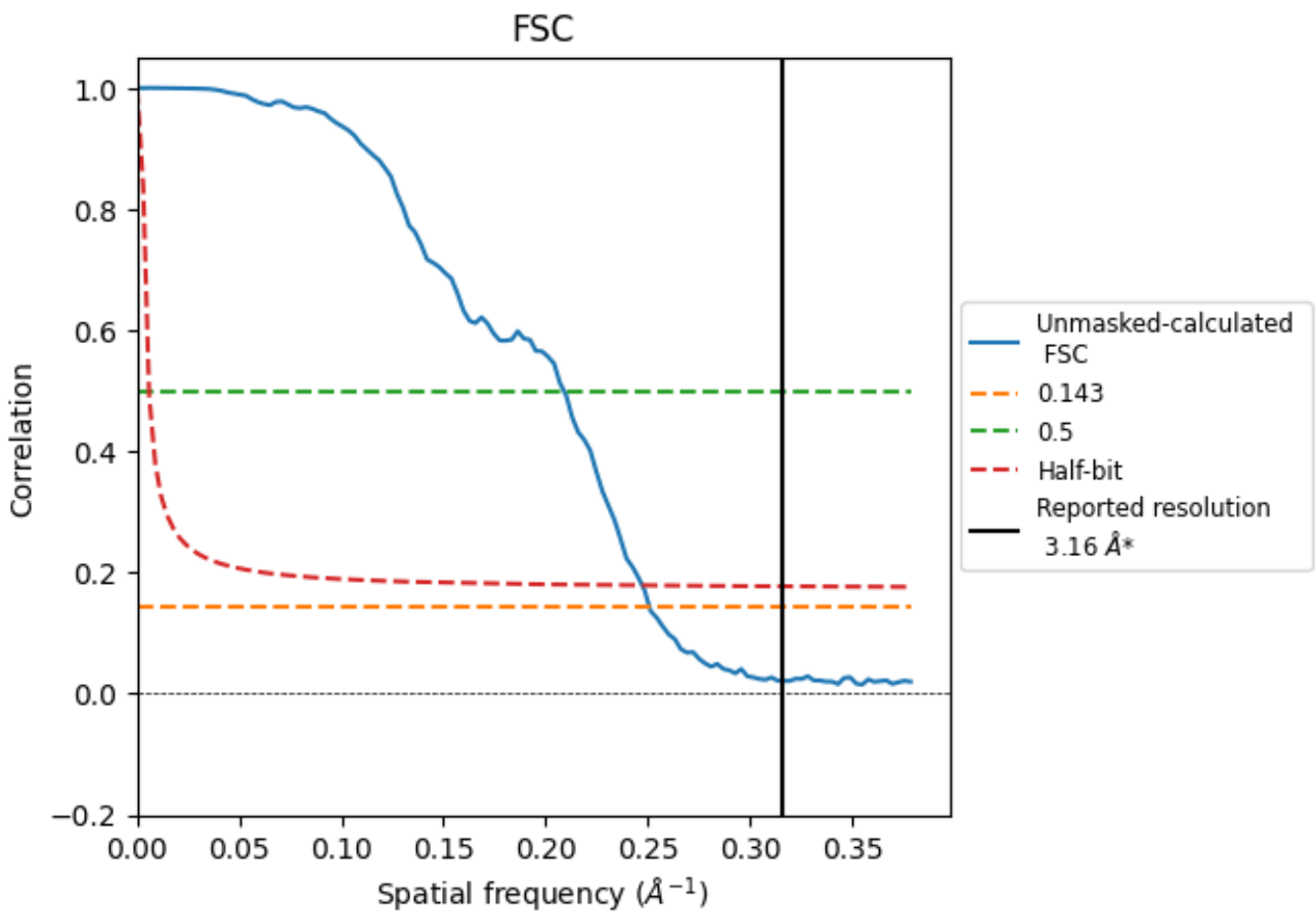


*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

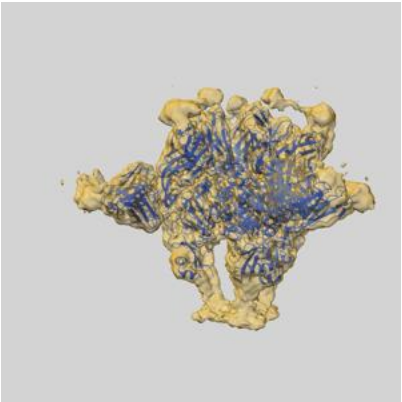
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	4.78	4.04

*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 3.99 differs from the reported value 3.16 by more than 10 %

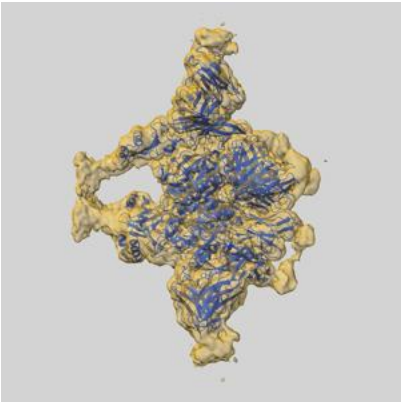
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-75814 and PDB model 11LR. Per-residue inclusion information can be found in section 3 on page 10.

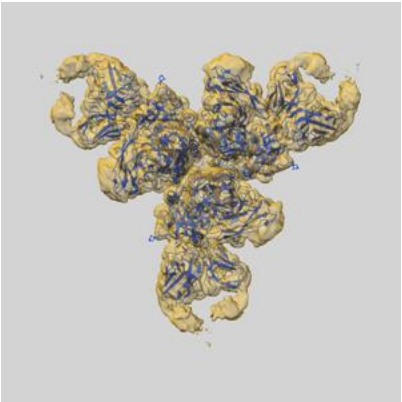
9.1 Map-model overlay (i)



X



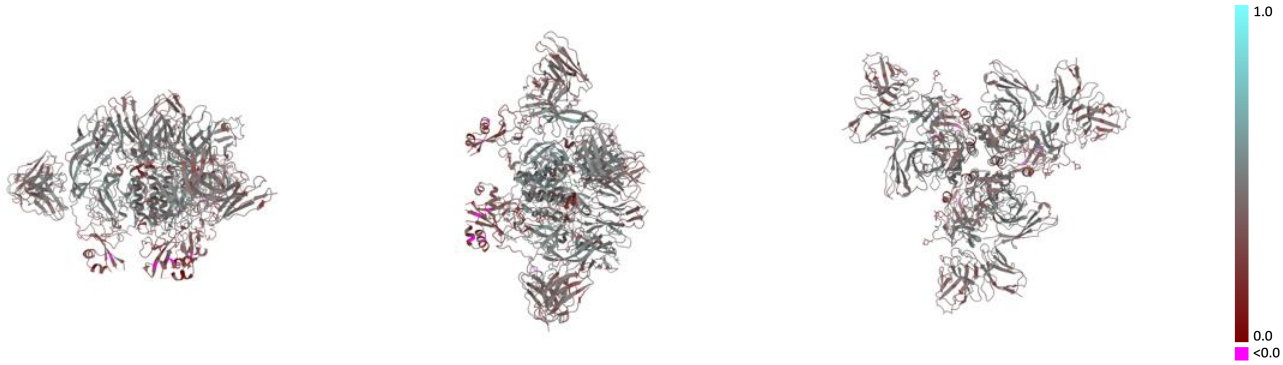
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

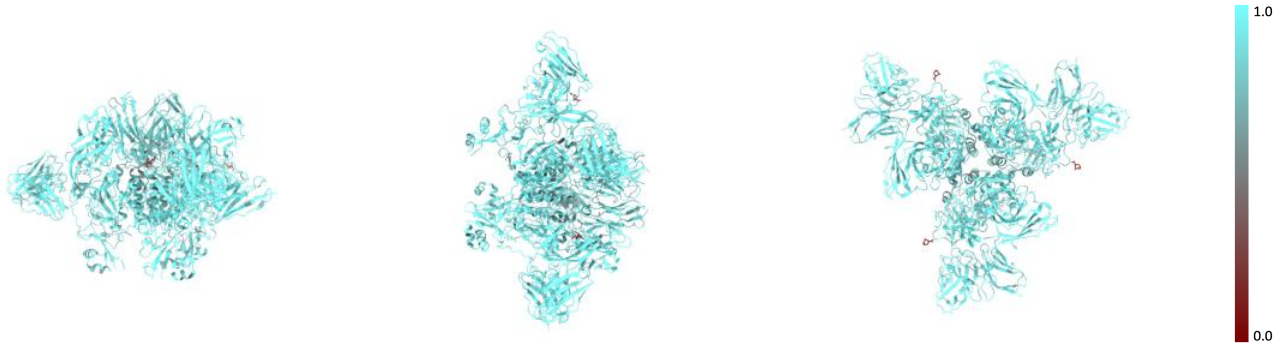
9.2 Q-score mapped to coordinate model (i)



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.

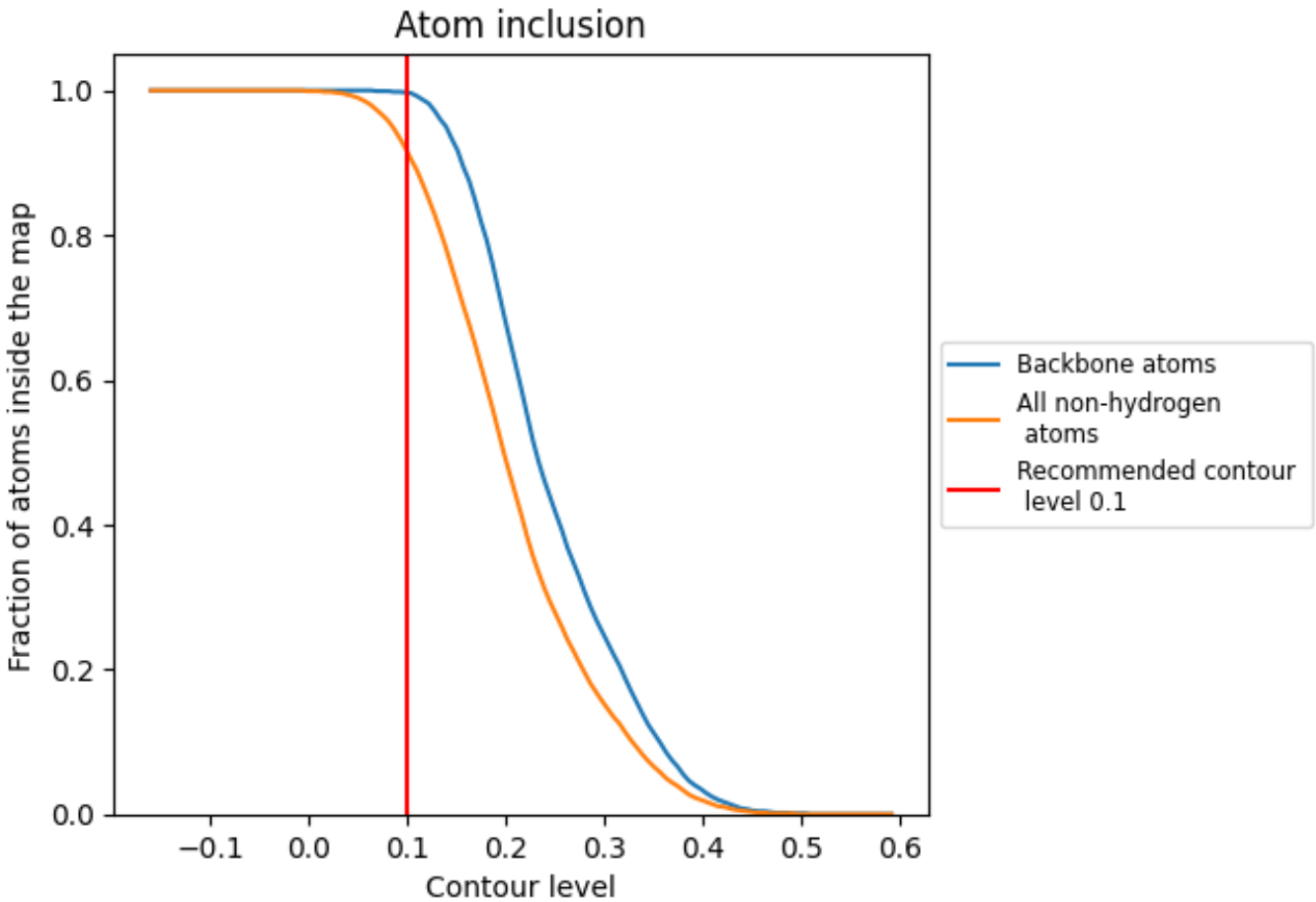
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9160	0.4220
A	0.9080	0.4220
B	0.9100	0.4200
C	0.9110	0.4220
D	0.8970	0.4220
E	0.9430	0.4560
F	0.8950	0.4230
G	0.9430	0.4560
H	0.9000	0.4250
I	0.9440	0.4580
J	0.9090	0.4070
K	0.9270	0.4030
L	0.9100	0.4080
M	0.9300	0.4010
N	0.9100	0.4060
o	0.9260	0.4000