



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 12:13 AM UTC

PDB ID : 7V3L / pdb_00007v3l
EMDB ID : EMD-31683
Title : MERS S ectodomain trimer in complex with neutralizing antibody 6516
Authors : Wang, X.; Zhao, J.; Wang, Z.; Wang, Y.; Zeng, J.
Deposited on : 2021-08-10
Resolution : 3.47 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:

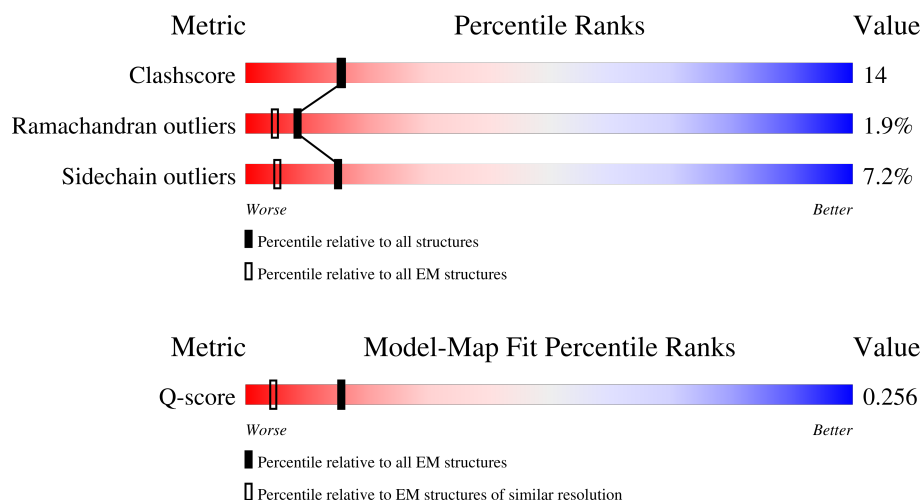
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

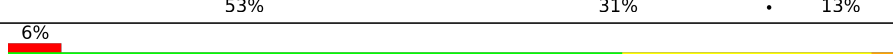
The reported resolution of this entry is 3.47 Å.

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.



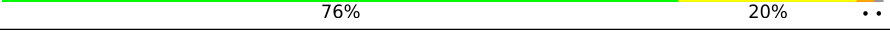
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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

Mol	Chain	Length	Quality of chain
1	A	1290	
1	B	1290	
1	C	1290	
2	D	226	

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Mol	Chain	Length	Quality of chain
2	F	226	 7% 69% 28% .
2	H	226	 2% 72% 26% .
3	E	215	 1% 78% 19% .
3	G	215	 2% 77% 20% .
3	I	215	 2% 76% 20% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36238 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1131	Total	C	N	O	S	1	0
			8737	5550	1441	1695	51		
1	B	1135	Total	C	N	O	S	1	0
			8785	5579	1453	1702	51		
1	C	1126	Total	C	N	O	S	1	0
			8719	5536	1442	1690	51		

- Molecule 2 is a protein called antibody H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	226	Total	C	N	O	S	0	0
			1688	1063	279	337	9		
2	F	226	Total	C	N	O	S	0	0
			1688	1063	279	337	9		
2	H	226	Total	C	N	O	S	0	0
			1681	1057	279	336	9		

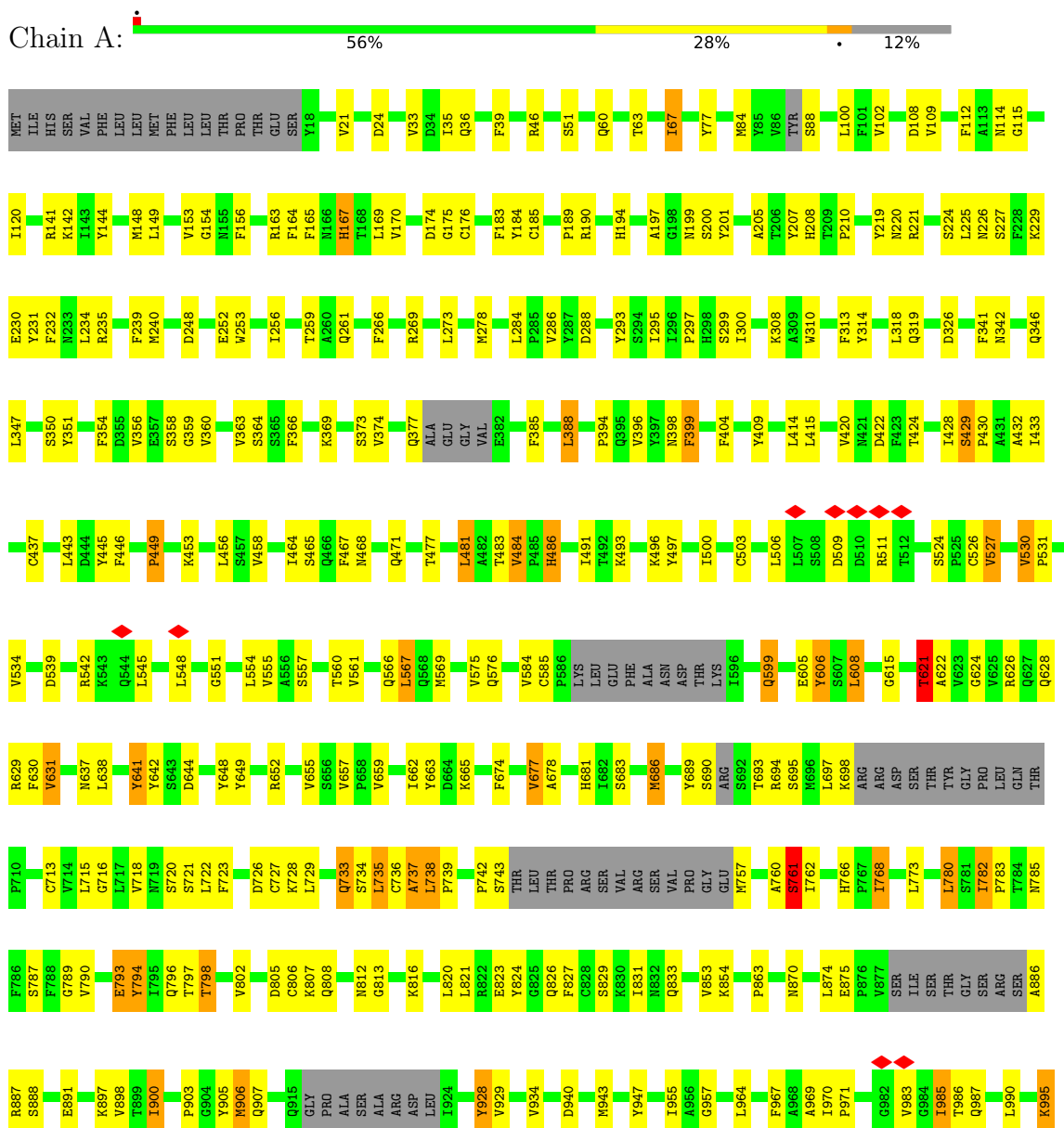
- Molecule 3 is a protein called antibody L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	214	Total	C	N	O	S	0	0
			1651	1037	277	332	5		
3	G	214	Total	C	N	O	S	0	0
			1651	1037	277	332	5		
3	I	212	Total	C	N	O	S	0	0
			1638	1030	275	328	5		

3 Residue-property plots

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: Spike glycoprotein

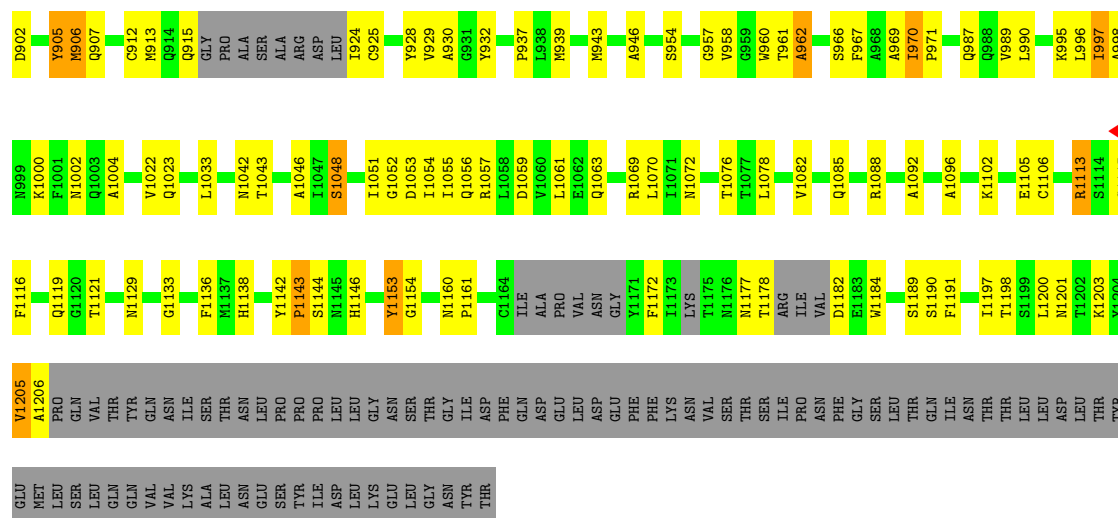


T961	L1075	E1183	SER
L964	T1076	W1184	LEU
S965	T1077	S1185	THR
S966	L1078	Y1186	GLN
F967	A1092	Y1192	ILE
A968	N1104	P1196	ASN
Y983	K1108	S1199	THR
G984	A1109	L1200	LEU
L990	Q1110	N1201	ASP
Q994	K1111	Y1204	LEU
K995	K1112	Y1205	THR
L996	R1113	A1206	PRO
Y997	S1114	PRO	GLU
A998	F1115	LEU	THR
M1008	F1116	GLN	LEU
N1016	G1117	VAL	SER
F1019	G1118	THR	GLN
Q1020	Q1119	TYR	ALA
K1021	G1120	GLN	LEU
N1027	T1121	VAL	ASN
P1131	H1122	LYS	GLY
N1028	I1123	ILE	LEU
N1029	V1124	THR	ASN
A1030	S1125	LEU	GLU
Q1031	A1130	PRO	TYR
A1032	M132	PRO	ILE
L1033	G1133	LEU	ASP
S1034	L1134	LEU	LEU
K1035	Y1135	GLY	LYS
L1040	F1136	ASN	GLU
T1043	M137	SER	LEU
G1045	H1138	GLY	THR
S1050	Y1141	ILE	ASN
I1051	Y1142	ASP	TYR
D1052	P1143	PHE	THR
D1053	S1144	GLN	
I1054	G1154	ASP	
I1055	LEU	LEU	
Q1056	M1160	ASP	
R1057	P1161	GLU	
L1058	G1164	PHE	
E1062	T1165	LYS	
Q1063	A1166	ASN	
I1067	P1167	VAL	
L1179	N1169	SER	
I1180	G1170	THR	
V1181	T1170	ILE	
D1182	R1179	PRO	
	I1180	ASN	
	V1181	PHE	
	D1182	GLY	

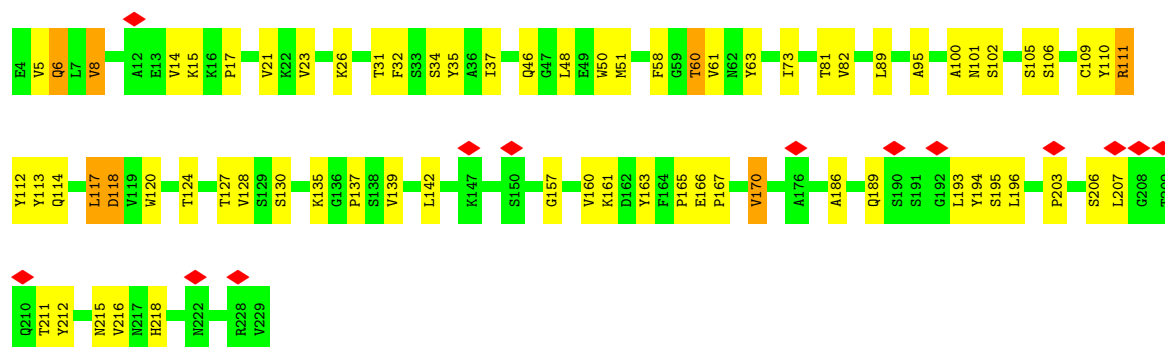
• Molecule 1: Spike glycoprotein

Chain C:  53% 31% 13%

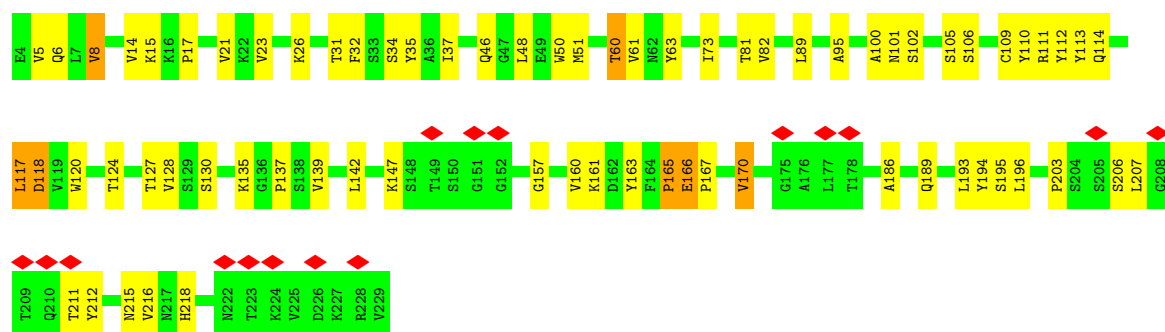
Y86	D174	V375	T477	L567	V649	Q727	D805
TYR	G175	E376	T477	Q568	C650	K728	Q809
S88	L180	Q377	L480	Y569	L651	G732	Y809
A89	R181	ALA	A481	V575	A653	L735	V810
G90	T257	GLY	A482	Q576	S656	C736	G813
PHE	H91	VAL	T483	V584	K655	A737	F814
LEU	A92	E382	V484	C585	V659	D740	E818
LEU	T95	F385	H486	L586	K665	T741	Q819
MET	C185	F385	H486	LYS	L673	T744	R822
PHE	T96	L388	T490	LEU	S676	THR	I831
LEU	P97	L388	T491	GLY	VAL	PRO	Q842
LEU	Q98	L388	T491	PHE	A678	ARG	V845
THR	K99	P394	T492	ALA	C679	VAL	L849
PRO	L100	Q395	T492	ASN	S680	ARG	V853
THR	F101	V396	K493	THR	H681	VAL	I861
THR	Y105	N398	K496	X595	Y689	GLY	I862
GLU	K110	F399	Y497	L596	S690	GLY	R865
GLU	Y18	F404	Y500	A597	S691	THR	G866
Y18	V21	Y409	C503	Q599	S692	THR	G867
V21	K27	Y409	L506	C603	S692	THR	D868
K27	C30	Y201	D509	V603	S692	THR	F869
C30	E32	Y202	D509	V603	S692	THR	T872
E32	V33	F204	R510	Y606	S692	THR	E875
V33	D34	Y206	R511	G614	S692	THR	P876
D34	I131	Y207	R511	R614	S692	THR	V877
I131	Q36	Y207	R511	G615	S692	THR	SER
Q36	Q37	Y207	R511	G615	S692	THR	ILE
Q37	F40	Y207	R511	G615	S692	THR	THR
F40	S137	Y207	R511	G615	S692	THR	GLY
S137	A138	Y207	R511	G615	S692	THR	ARG
A138	T139	Y207	R511	G615	S692	THR	PRO
T139	I140	Y207	R511	G615	S692	THR	LEU
I140	R141	Y207	R511	G615	S692	THR	GLN
R141	K142	Y207	R511	G615	S692	THR	THR
K142	P145	Y207	R511	G615	S692	THR	TYR
P145	L57	Y207	R511	G615	S692	THR	GLY
L57	F58	Y207	R511	G615	S692	THR	PRO
F58	P59	Y207	R511	G615	S692	THR	LEU
P59	D60	Y207	R511	G615	S692	THR	GLN
D60	G61	Y207	R511	G615	S692	THR	THR
G61	R62	Y207	R511	G615	S692	THR	GLY
R62	T63	Y207	R511	G615	S692	THR	ARG
T63	V64	Y207	R511	G615	S692	THR	SER
V64	S65	Y207	R511	G615	S692	THR	ARG
S65	R66	Y207	R511	G615	S692	THR	ARG
R66	T67	Y207	R511	G615	S692	THR	ARG
T67	Y71	Y207	R511	G615	S692	THR	ARG
Y71	Q78	Y207	R511	G615	S692	THR	ARG
Q78	H81	Y207	R511	G615	S692	THR	ARG
H81	M84	Y207	R511	G615	S692	THR	ARG
M84	L171	Y207	R511	G615	S692	THR	ARG
L171	L172	Y207	R511	G615	S692	THR	ARG
L172	P173	Y207	R511	G615	S692	THR	ARG
P173	Y85	Y207	R511	G615	S692	THR	ARG
Y85		Y207	R511	G615	S692	THR	ARG



- Molecule 2: antibody H

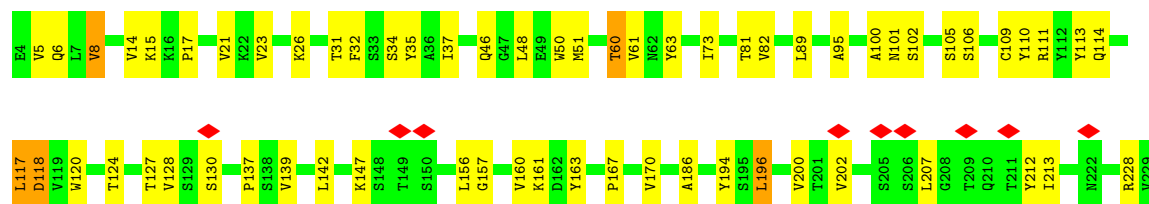


- Molecule 2: antibody H

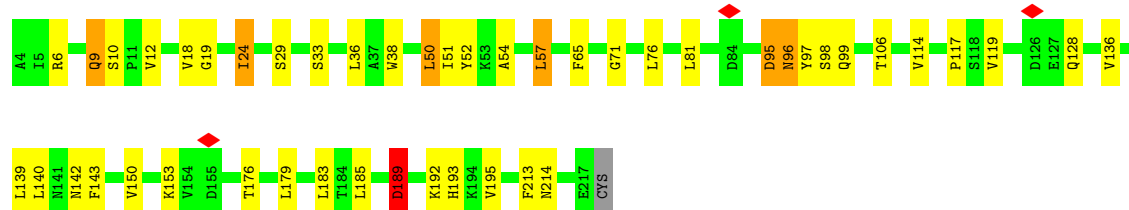
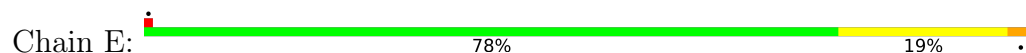


- Molecule 2: antibody H

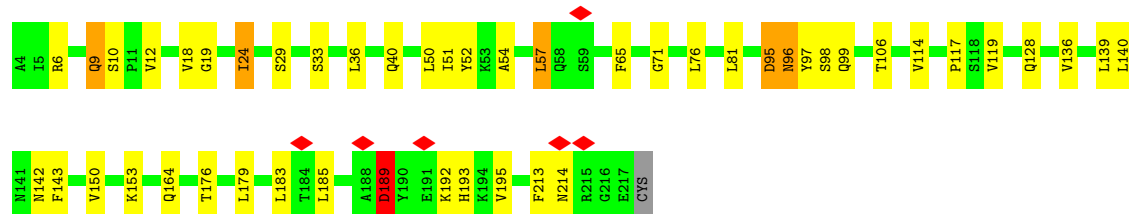
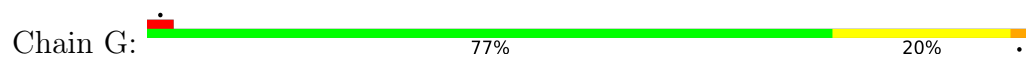




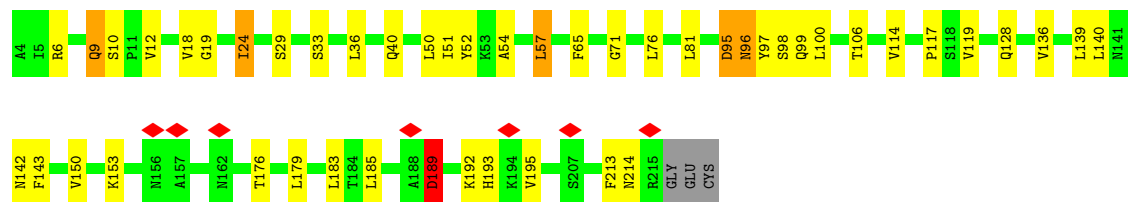
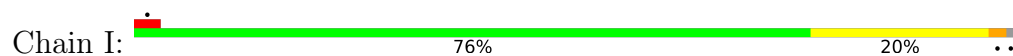
• Molecule 3: antibody L



• Molecule 3: antibody L



• Molecule 3: antibody L



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1289518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.86	5/8931 (0.1%)	1.10	20/12136 (0.2%)
1	B	0.81	5/8981 (0.1%)	1.06	22/12206 (0.2%)
1	C	0.80	4/8912 (0.0%)	1.03	15/12105 (0.1%)
2	D	1.06	1/1729 (0.1%)	1.19	2/2357 (0.1%)
2	F	1.02	0/1729	1.19	1/2357 (0.0%)
2	H	1.03	0/1721	1.18	1/2346 (0.0%)
3	E	1.02	0/1687	1.26	3/2291 (0.1%)
3	G	1.02	0/1687	1.26	3/2291 (0.1%)
3	I	1.03	0/1674	1.26	3/2274 (0.1%)
All	All	0.89	15/37051 (0.0%)	1.11	70/50363 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	111	ARG	C-N	10.22	1.48	1.33
1	A	449	PRO	C-N	7.93	1.44	1.34
1	B	449	PRO	C-N	7.92	1.44	1.34
1	C	449	PRO	C-N	7.91	1.44	1.34
1	C	575	VAL	C-N	7.43	1.43	1.33

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	714	VAL	N-CA-C	-11.20	102.71	112.12
1	A	997	ILE	N-CA-C	-10.08	99.89	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	695	SER	N-CA-C	-9.21	102.18	113.97
2	F	165	PRO	N-CA-C	8.60	125.48	113.53
1	B	692	SER	N-CA-C	-8.57	103.33	112.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51[A]	SER	Mainchain
1	A	51[B]	SER	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8737	0	8422	271	0
1	B	8785	0	8501	314	0
1	C	8719	0	8414	319	0
2	D	1688	0	1636	39	0
2	F	1688	0	1636	40	0
2	H	1681	0	1629	35	0
3	E	1651	0	1615	27	0
3	G	1651	0	1615	25	0
3	I	1638	0	1606	24	0
All	All	36238	0	35074	1031	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 14.

The worst 5 of 1031 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ILE:H	1:A:1181:VAL:HG21	1.50	0.77
1:B:189:PRO:HB2	1:B:197:ALA:HB2	1.66	0.77
1:A:683:SER:H	1:A:686:MET:HG2	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:LEU:HD21	1:C:1184:TRP:HB2	1.67	0.76
1:B:1040:LEU:HD22	1:B:1077:THR:HB	1.67	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1108/1290 (86%)	977 (88%)	117 (11%)	14 (1%)	9	39
1	B	1118/1290 (87%)	957 (86%)	132 (12%)	29 (3%)	4	27
1	C	1103/1290 (86%)	938 (85%)	135 (12%)	30 (3%)	4	27
2	D	224/226 (99%)	203 (91%)	18 (8%)	3 (1%)	9	39
2	F	224/226 (99%)	202 (90%)	18 (8%)	4 (2%)	6	33
2	H	224/226 (99%)	206 (92%)	15 (7%)	3 (1%)	9	39
3	E	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	24	58
3	G	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	24	58
3	I	210/215 (98%)	196 (93%)	12 (6%)	2 (1%)	12	44
All	All	4635/5193 (89%)	4075 (88%)	473 (10%)	87 (2%)	8	32

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	737	ALA
1	A	995	LYS
1	A	1153	TYR
1	A	1181	VAL
1	B	731	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	970/1118 (87%)	893 (92%)	77 (8%)	11	36
1	B	978/1118 (88%)	913 (93%)	65 (7%)	15	42
1	C	969/1118 (87%)	921 (95%)	48 (5%)	22	48
2	D	191/191 (100%)	175 (92%)	16 (8%)	10	34
2	F	191/191 (100%)	174 (91%)	17 (9%)	9	33
2	H	190/191 (100%)	173 (91%)	17 (9%)	9	33
3	E	188/189 (100%)	170 (90%)	18 (10%)	8	30
3	G	188/189 (100%)	171 (91%)	17 (9%)	9	32
3	I	187/189 (99%)	170 (91%)	17 (9%)	9	32
All	All	4052/4494 (90%)	3760 (93%)	292 (7%)	15	38

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	51	MET
3	I	140	LEU
2	F	170	VAL
2	H	8	VAL
1	B	626	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1042	ASN
2	F	6	GLN
1	C	1119	GLN
2	D	210	GLN
3	G	41	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

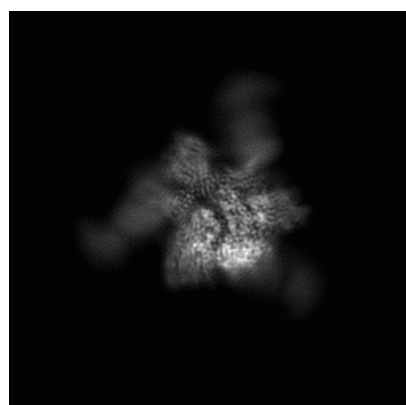
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31683. These allow visual inspection of the internal detail of the map and identification of artifacts.

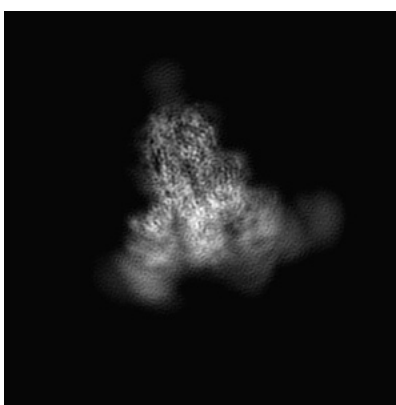
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

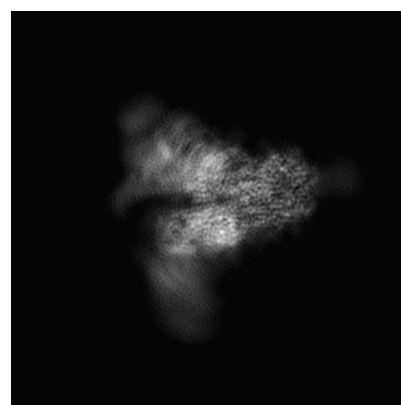
6.1.1 Primary map



X



Y

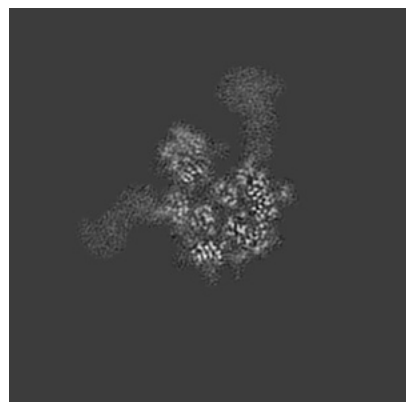


Z

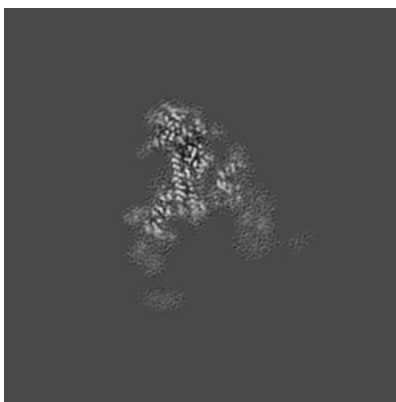
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

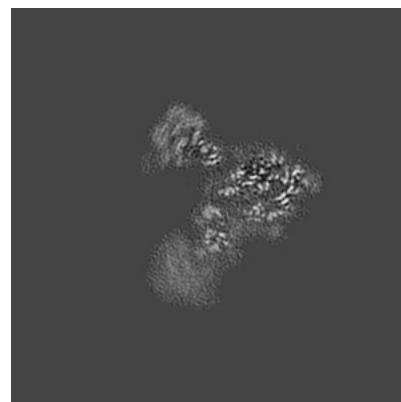
6.2.1 Primary map



X Index: 160



Y Index: 160

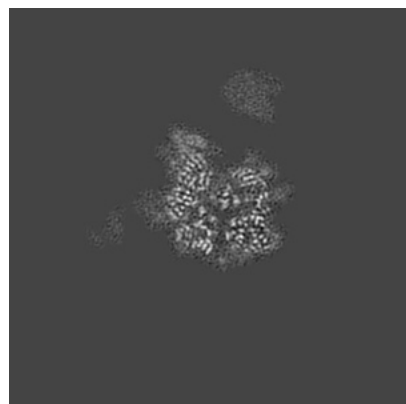


Z Index: 160

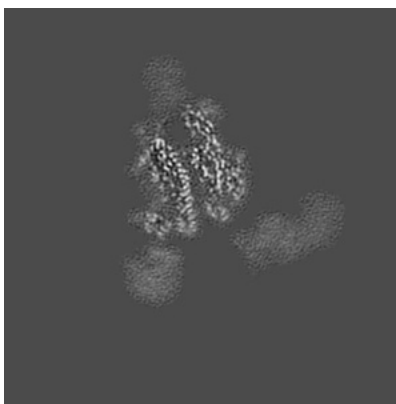
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

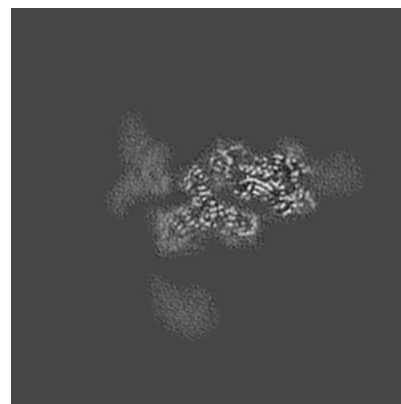
6.3.1 Primary map



X Index: 167



Y Index: 179

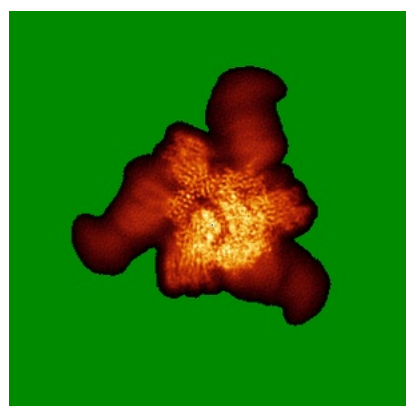


Z Index: 127

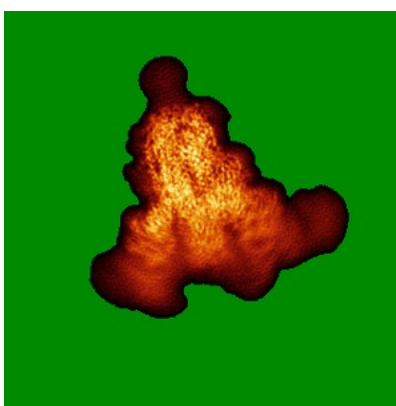
The images above show the largest variance slices of the map in three orthogonal directions.

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

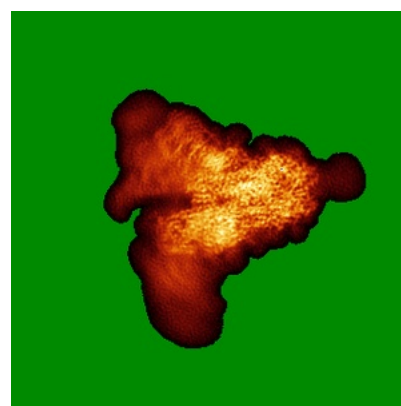
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

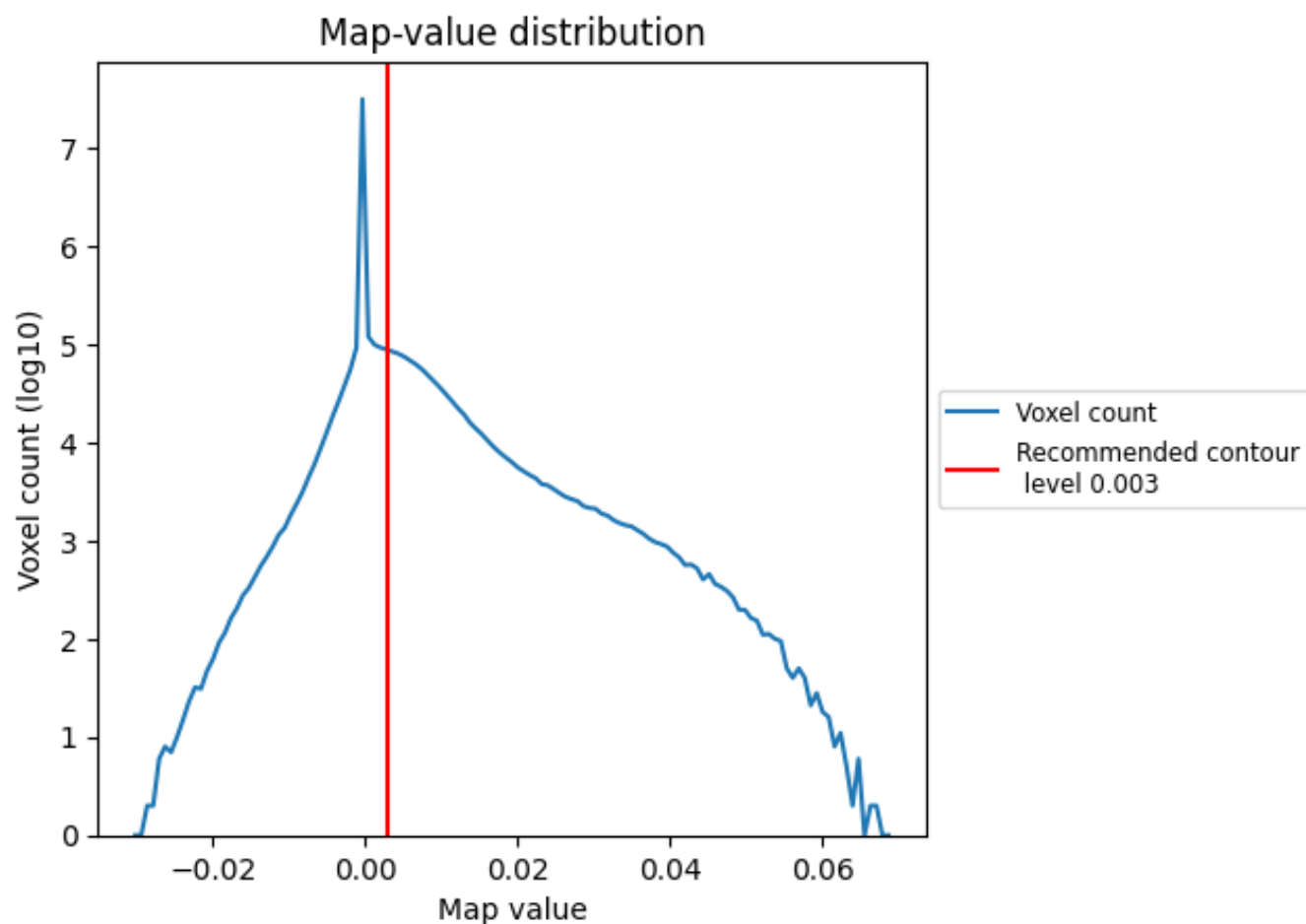
6.6 Mask visualisation

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

7 Map analysis [i](#)

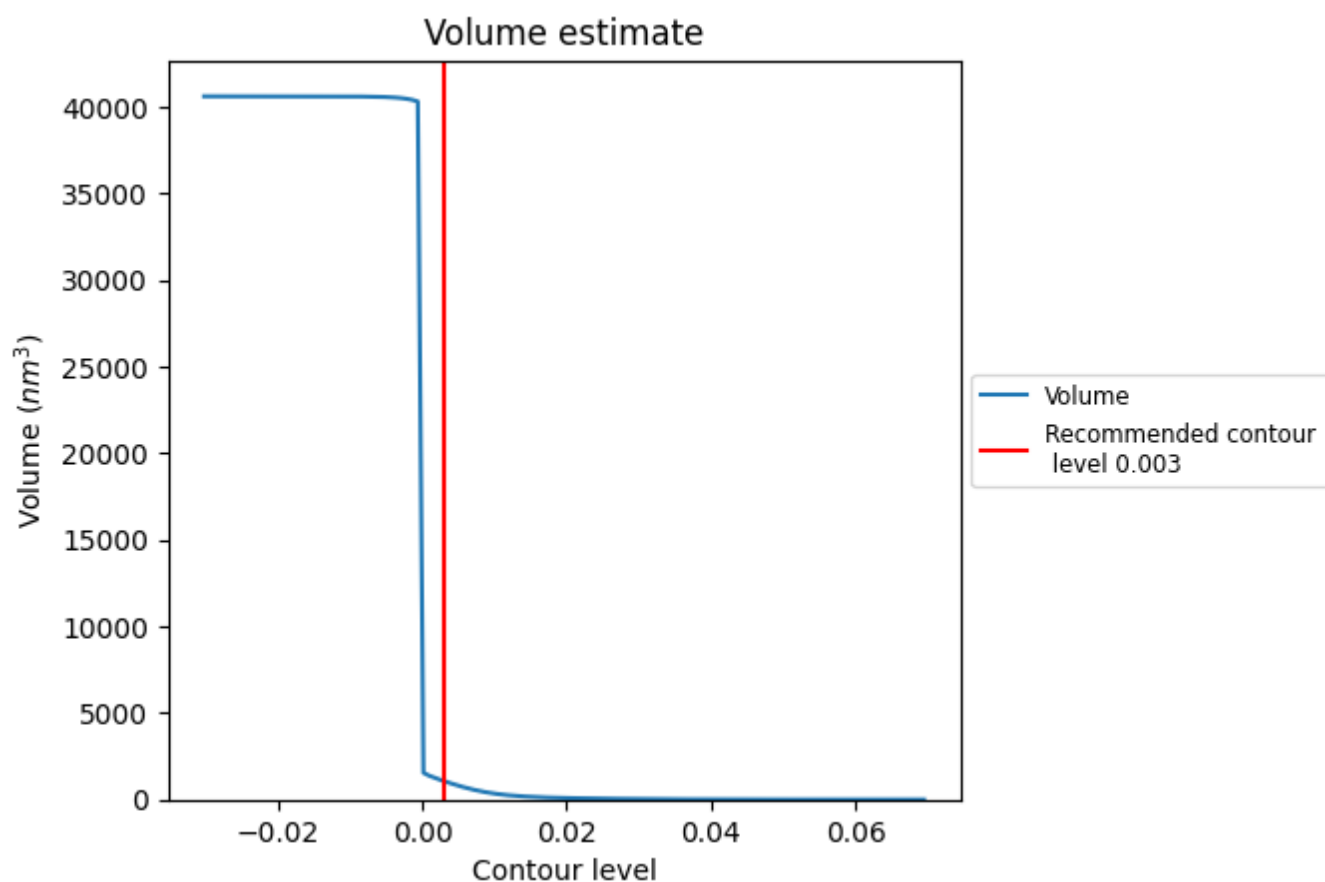
This section contains the results of statistical analysis of the map.

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.

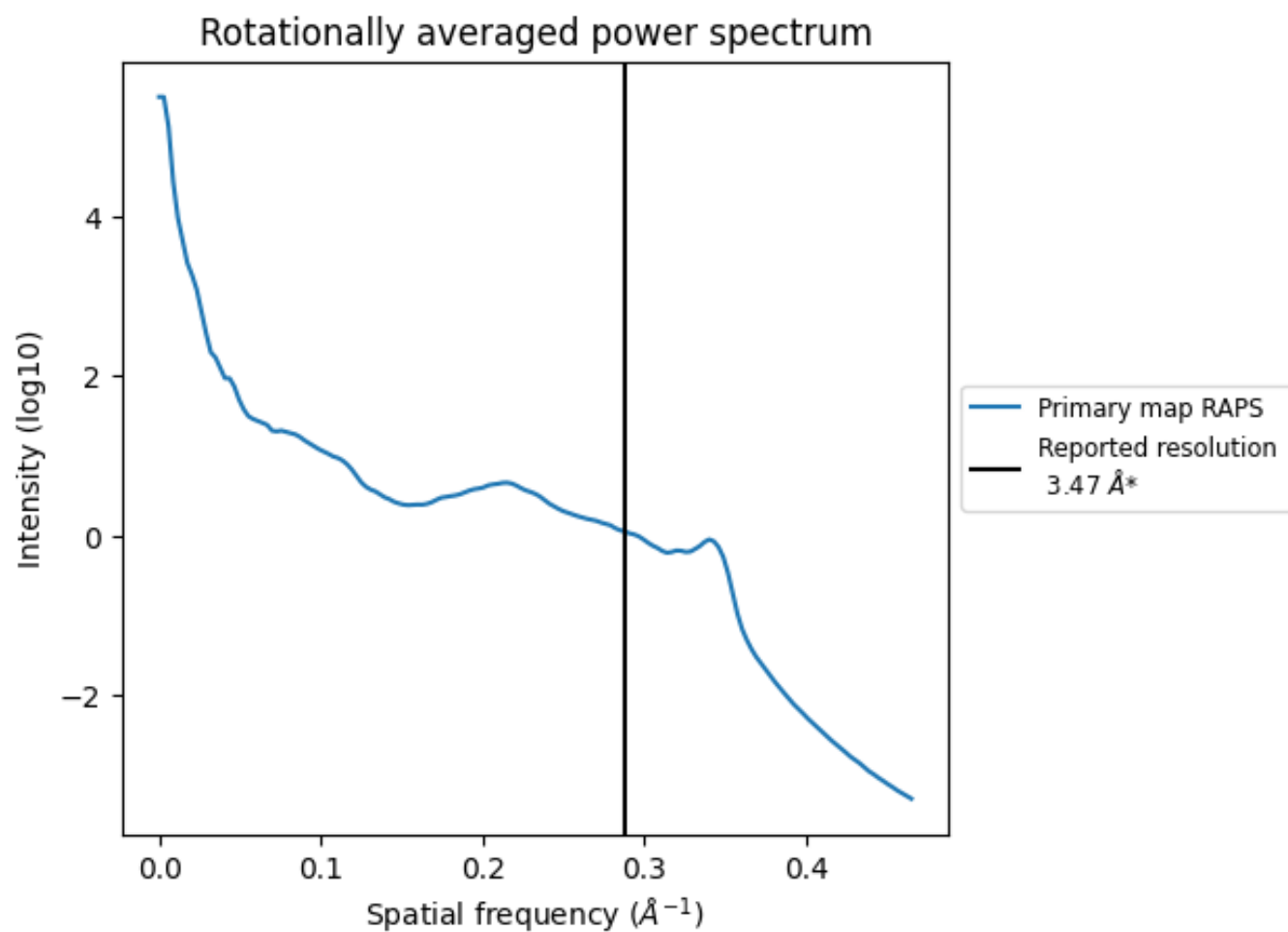
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1070 nm³; this corresponds to an approximate mass of 967 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

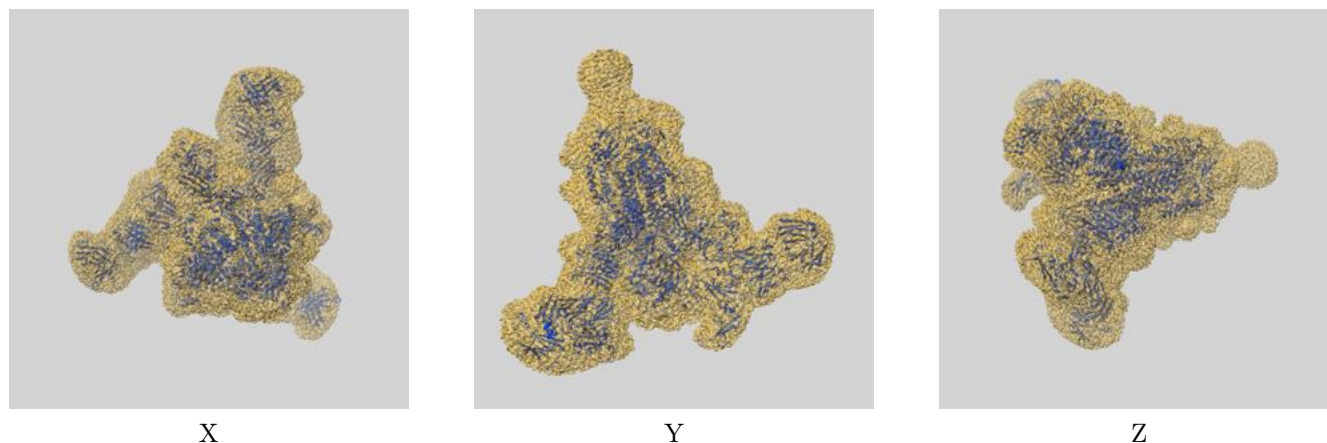
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

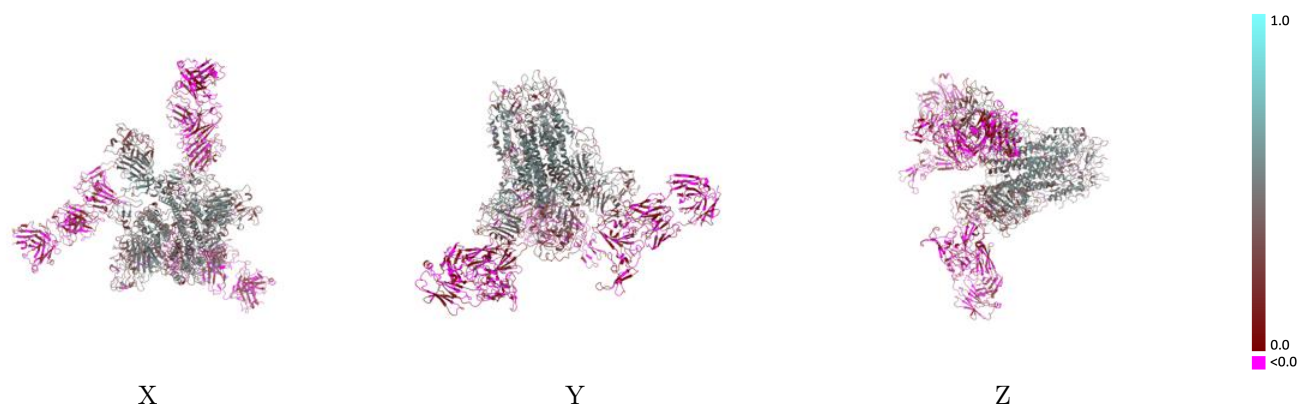
This section contains information regarding the fit between EMDB map EMD-31683 and PDB model 7V3L. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



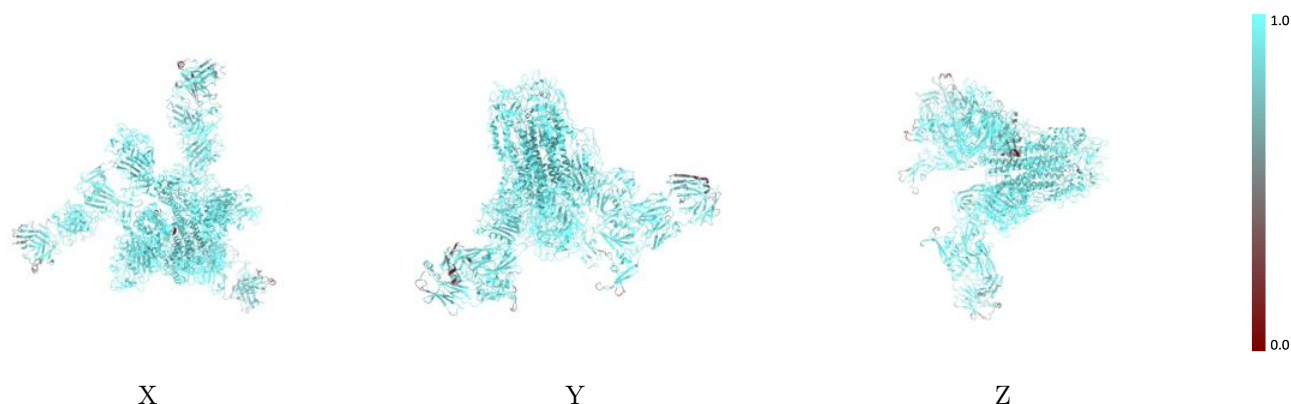
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



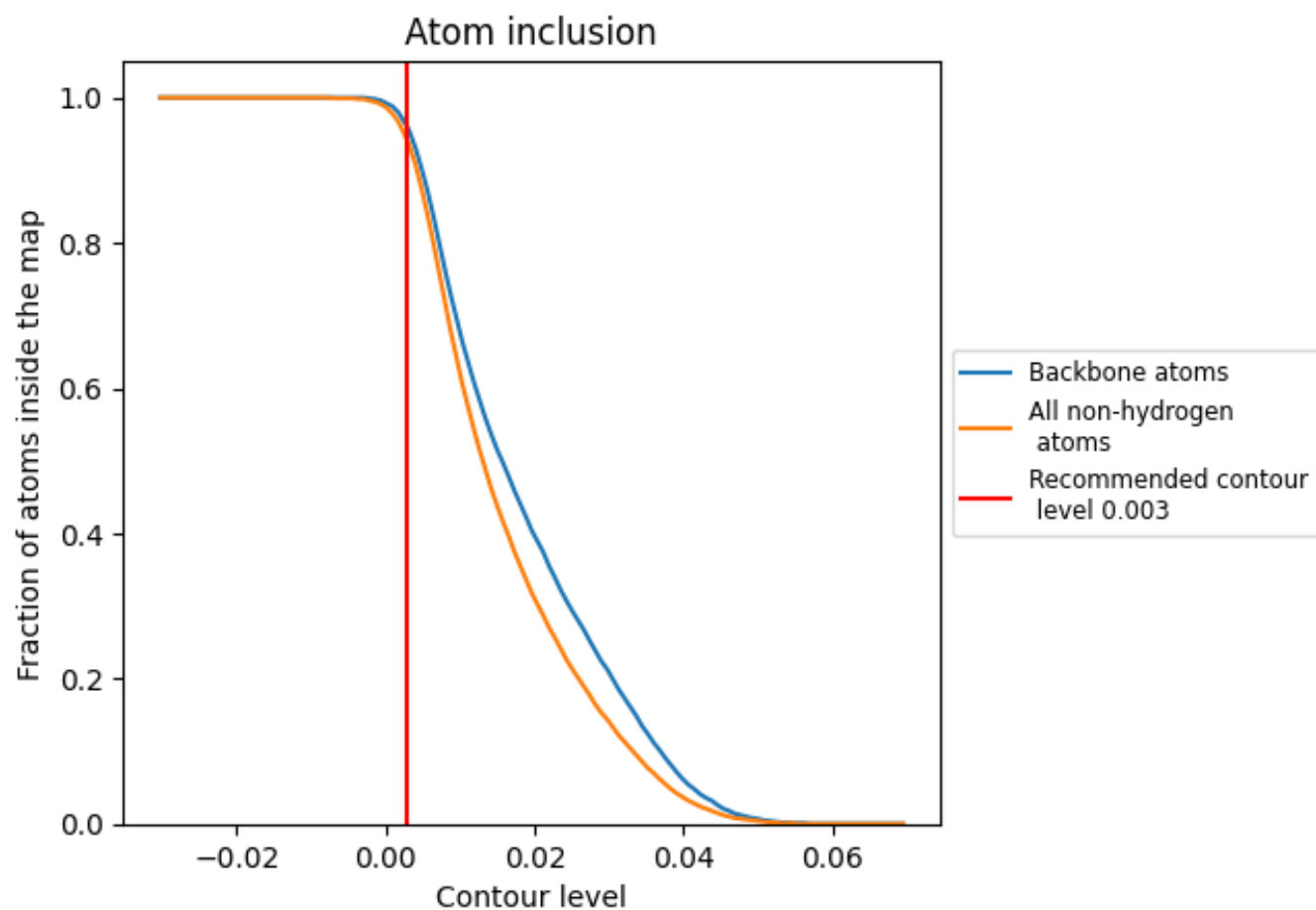
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.2560
A	0.9640	0.3380
B	0.9630	0.3520
C	0.9680	0.3390
D	0.8610	0.0170
E	0.8950	0.0350
F	0.8510	0.0400
G	0.8600	0.0300
H	0.9060	0.0200
I	0.8800	0.0120

1.0

0.0

<0.0