

Full wwPDB EM Validation Report (i)

Oct 7, 2023 – 01:08 PM EDT

PDB ID : 8SR0

EMDB ID : EMD-40716

Title: CryoEM structure of a therapeutic antibody (favezelimab) bound to human

LAG3 local refined

Authors: Mishra, A.K.; Shahid, S.; Karade, S.S.; Mariuzza, R.A.

Deposited on : 2023-05-05

Resolution : 3.53 Å(reported)

Based on initial model : 7TZG

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 (i)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50

Mogul : 1.8.5 (274361), CSD as541be (2020)

MolProbity : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ: 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

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 3.53 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11440 atoms, of which 5452 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 Lymphocyte activation gene 3 protein.

	\mathbf{Mol}	Chain	Residues			Atom	.S			AltConf	Trace	
	1	V	182	Total	С	Н	N	О	S	0	0	
	1	Λ	102	2479	829	1169	243	232	6	U	U	
İ	1	D	181	Total	С	Н	N	О	S	0	0	1
	1	D	101	2493	820	1187	249	231	6	U	U	

• Molecule 2 is a protein called favezelimab Fab heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace		
2	V	119	Total	С	Н	N	О	S	0	0
2	1	119	1743	570	843	156	170	4	0	
2	Н	116	Total	С	Н	N	О	S	0	0
2	11	110	1553	529	721	142	157	4	U	U

• Molecule 3 is a protein called favezelimab Fab light chain.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
2	7	109	Total	С	Н	N	О	S	0	0
3		109	1568	498	758	138	171	3	0	
2	Т	109	Total	С	Н	N	О	S	0	0
3	ь	109	1550	494	748	137	168	3	U	U

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues		At	oms			AltConf	
1	v	1	Total	С	Н	N	О	0	
4	Λ	1	27	8	13	1	5	0	
1	D	1	Total	С	Н	N	О	0	
4	ש	1	27	8	13	1	5		

MolProbity failed to run properly - this section is therefore empty.



3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.698	Depositor
Minimum map value	-1.860	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor



4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

2 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	Т	ype Chain Res Link		Bo	ond leng	$ ag{ths}$	Bond angles			
MIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	601	-	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	X	601	-	14,14,15	0.24	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	601	-	-	0/6/23/26	0/1/1/1
4	NAG	X	601	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	601	NAG	O5-C5-C6-O6
4	X	601	NAG	C8-C7-N2-C2
4	X	601	NAG	O7-C7-N2-C2
4	X	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



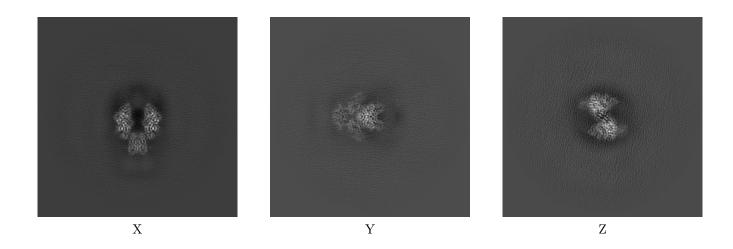
5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40716. These allow visual inspection of the internal detail of the map and identification of artifacts.

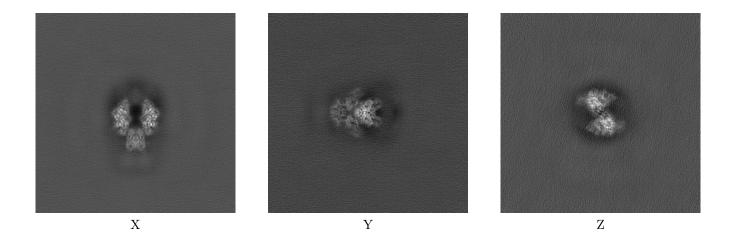
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections (i)

5.1.1 Primary map



5.1.2 Raw map



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

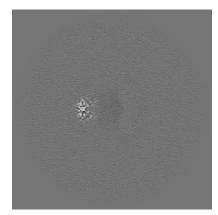


5.2 Central slices (i)

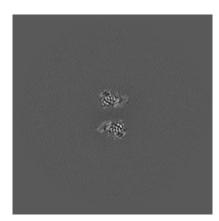
5.2.1 Primary map





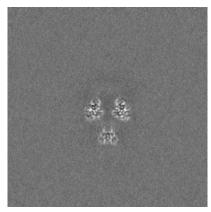


Y Index: 160

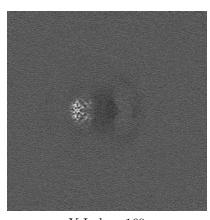


Z Index: 160

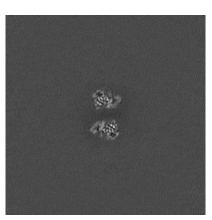
5.2.2 Raw map



X Index: 160



Y Index: 160



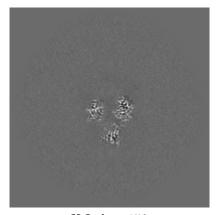
Z Index: 160

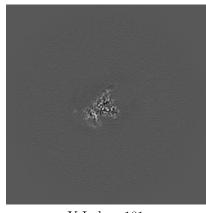
The images above show central slices of the map in three orthogonal directions.



5.3 Largest variance slices (i)

5.3.1 Primary map





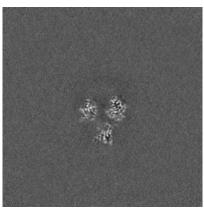


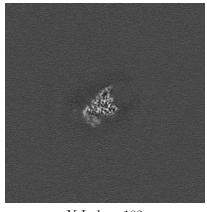
X Index: 156

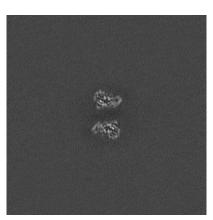
Y Index: 181

Z Index: 161

5.3.2 Raw map







X Index: 156

Y Index: 183

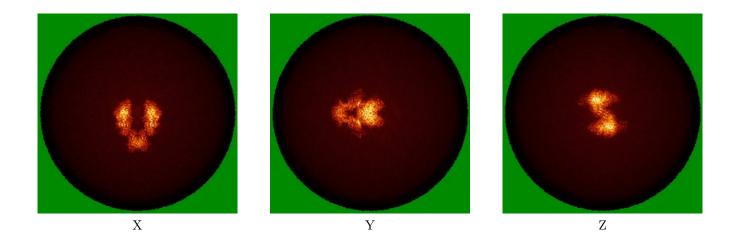
Z Index: 162

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

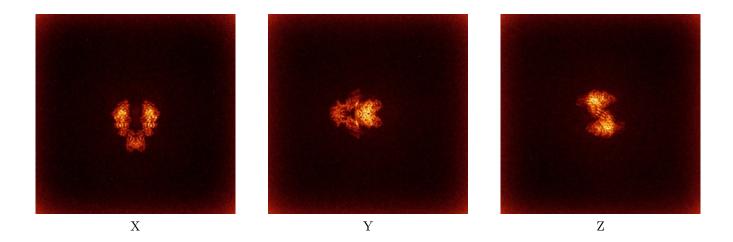


5.4 Orthogonal standard-deviation projections (False-color) (i)

5.4.1 Primary map



5.4.2 Raw map

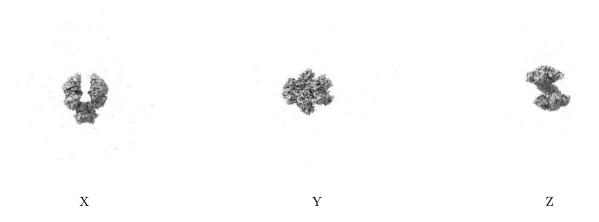


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



5.5 Orthogonal surface views (i)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



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.

5.6 Mask visualisation (i)

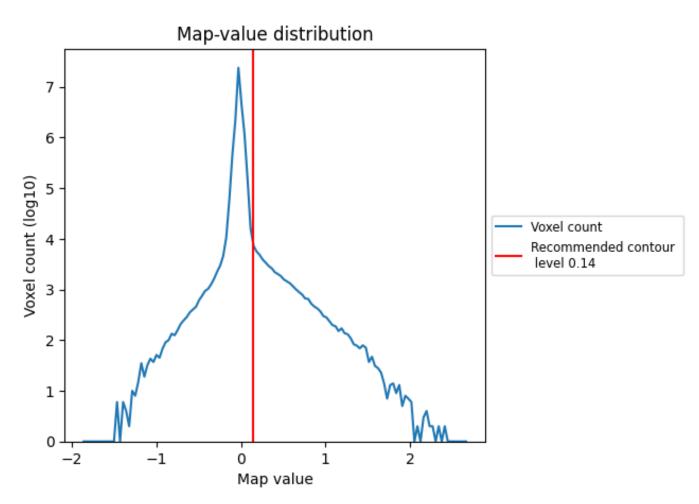
This section was not generated. No masks/segmentation were deposited.



6 Map analysis (i)

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

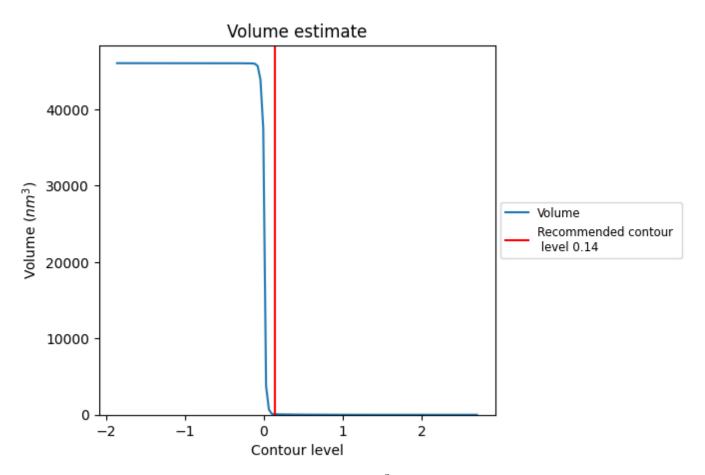
6.1 Map-value distribution (i)



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.



6.2 Volume estimate (i)

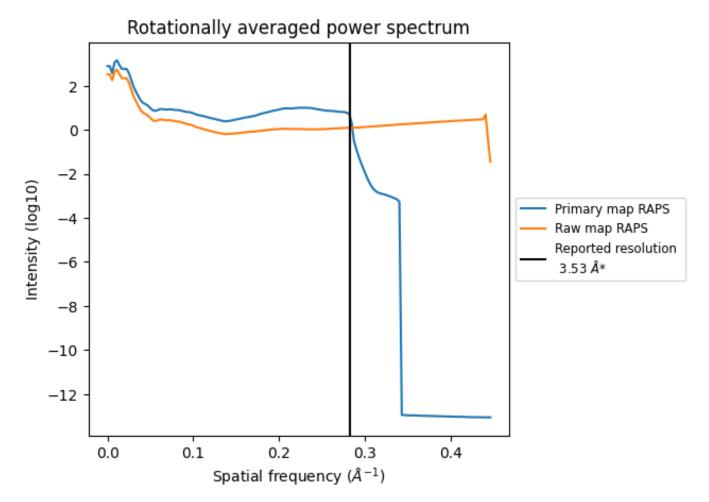


The volume at the recommended contour level is $75~\mathrm{nm^3}$; this corresponds to an approximate mass of $68~\mathrm{kDa}$.

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.



6.3 Rotationally averaged power spectrum (i)



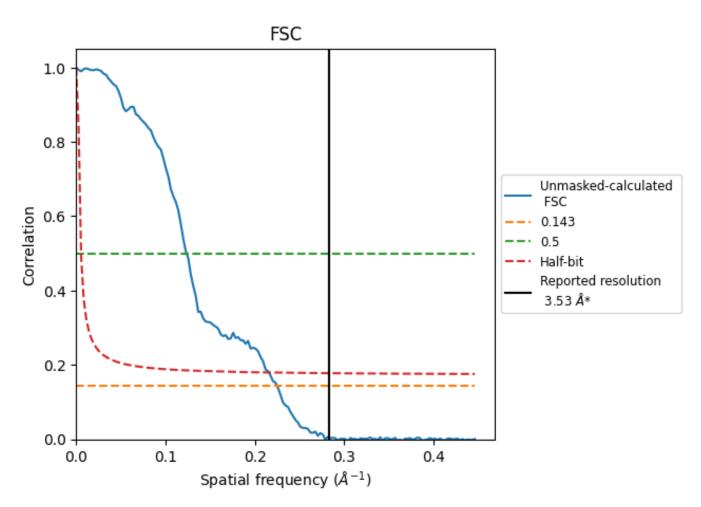
^{*}Reported resolution corresponds to spatial frequency of 0.283 $\rm \mathring{A}^{-1}$



7 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.

7.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.283 $\rm \mathring{A}^{-1}$



7.2 Resolution estimates (i)

Resolution estimate (Å)	Estim	Estimation criterion (FSC cut-off					
rtesolution estimate (A)	0.143	0.5	Half-bit				
Reported by author	3.53	-	-				
Author-provided FSC curve	-	-	-				
Unmasked-calculated*	4.44	8.09	4.63				

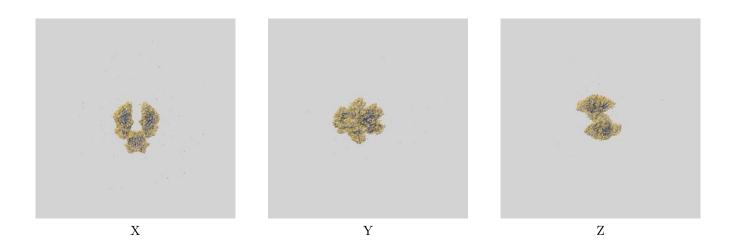
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.53 by more than 10 %



8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40716 and PDB model 8SR0. Per-residue inclusion information can be found in section ?? on page ??.

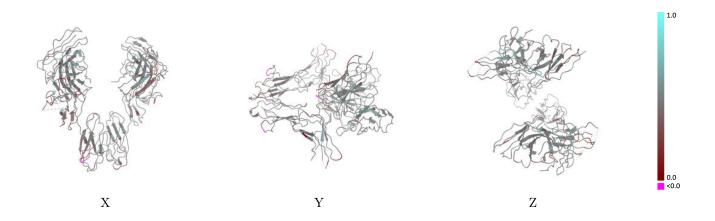
8.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.14 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.

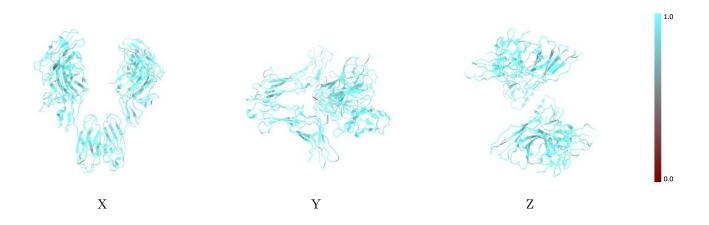


8.2 Q-score mapped to coordinate model (i)



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.

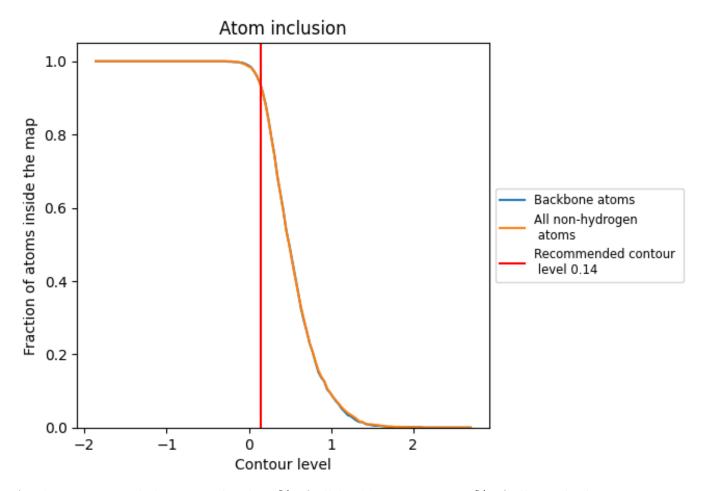
8.3 Atom inclusion mapped to coordinate model (i)



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 (0.14).



8.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.4660
D	0.9300	0.4460
Н	0.9470	0.4790
L	0.9470	0.4790
X	0.9240	0.4540
Y	0.9370	0.4640
Z	0.9520	0.4930



