



## wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 08:58 AM EST

PDB ID : 8CW9  
EMDB ID : EMD-27024  
Title : Prefusion-stabilized hMPV fusion protein bound to ADI-61026 and MPE8 Fabs  
Authors : Hsieh, C.-L.; McLellan, J.S.  
Deposited on : 2022-05-18  
Resolution : 3.46 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.31.2



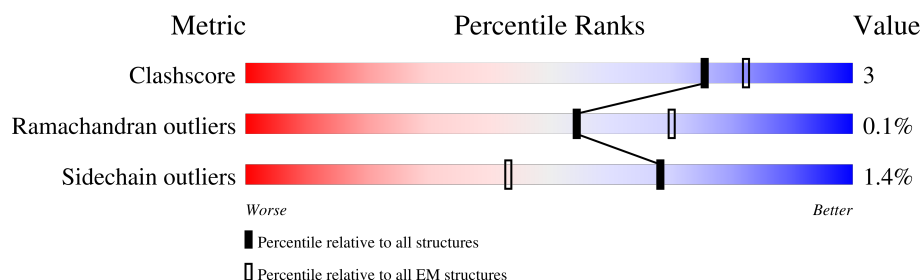
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



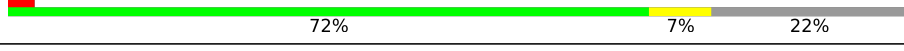
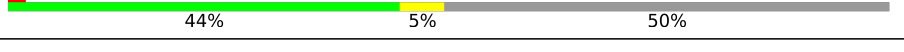
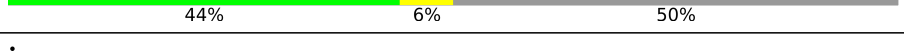
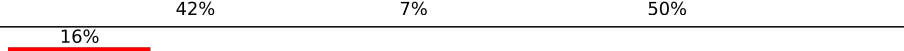
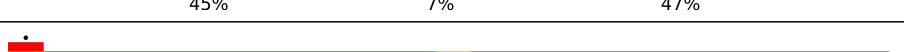
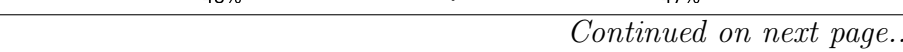
The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	551	
1	E	551	
1	F	551	
2	B	216	
2	M	216	
2	O	216	
3	C	228	
3	H	228	

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Mol	Chain	Length	Quality of chain
3	I	228	<div><div><div></div><div></div><div></div><div></div></div><div>16%45%8%47%</div></div>
4	D	214	<div><div><div></div><div></div><div></div><div></div></div><div>13%46%.50%</div></div>
4	K	214	<div><div><div></div><div></div><div></div><div></div></div><div>16%46%.50%</div></div>
4	L	214	<div><div><div></div><div></div><div></div><div></div></div><div>.45%.50%</div></div>
5	G	454	<div><div><div></div><div></div><div></div><div></div></div><div>.23%.73%</div></div>
5	J	454	<div><div><div></div><div></div><div></div><div></div></div><div>.25%.73%</div></div>
5	N	454	<div><div><div></div><div></div><div></div><div></div></div><div>.24%.73%</div></div>



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20229 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3260	2044	560	627	29		
1	E	430	Total	C	N	O	S	0	0
			3260	2044	560	627	29		
1	F	430	Total	C	N	O	S	0	0
			3260	2044	560	627	29		

There are 225 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	GLN	engineered mutation	UNP H6X1Z0
A	101	ARG	SER	engineered mutation	UNP H6X1Z0
A	110	CYS	LEU	engineered mutation	UNP H6X1Z0
A	127	CYS	THR	engineered mutation	UNP H6X1Z0
A	140	CYS	ALA	engineered mutation	UNP H6X1Z0
A	147	CYS	ALA	engineered mutation	UNP H6X1Z0
A	153	CYS	ASN	engineered mutation	UNP H6X1Z0
A	185	PRO	ALA	engineered mutation	UNP H6X1Z0
A	219	LYS	LEU	engineered mutation	UNP H6X1Z0
A	231	ILE	VAL	engineered mutation	UNP H6X1Z0
A	322	CYS	ASN	engineered mutation	UNP H6X1Z0
A	365	CYS	THR	engineered mutation	UNP H6X1Z0
A	453	GLN	GLU	engineered mutation	UNP H6X1Z0
A	463	CYS	VAL	engineered mutation	UNP H6X1Z0
A	491	GLY	-	expression tag	UNP H6X1Z0
A	492	GLY	-	expression tag	UNP H6X1Z0
A	493	GLY	-	expression tag	UNP H6X1Z0
A	494	SER	-	expression tag	UNP H6X1Z0
A	495	GLY	-	expression tag	UNP H6X1Z0
A	496	TYR	-	expression tag	UNP H6X1Z0
A	497	ILE	-	expression tag	UNP H6X1Z0
A	498	PRO	-	expression tag	UNP H6X1Z0
A	499	GLU	-	expression tag	UNP H6X1Z0
A	500	ALA	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	501	PRO	-	expression tag	UNP H6X1Z0
A	502	ARG	-	expression tag	UNP H6X1Z0
A	503	ASP	-	expression tag	UNP H6X1Z0
A	504	GLY	-	expression tag	UNP H6X1Z0
A	505	GLN	-	expression tag	UNP H6X1Z0
A	506	ALA	-	expression tag	UNP H6X1Z0
A	507	TYR	-	expression tag	UNP H6X1Z0
A	508	VAL	-	expression tag	UNP H6X1Z0
A	509	ARG	-	expression tag	UNP H6X1Z0
A	510	LYS	-	expression tag	UNP H6X1Z0
A	511	ASP	-	expression tag	UNP H6X1Z0
A	512	GLY	-	expression tag	UNP H6X1Z0
A	513	GLU	-	expression tag	UNP H6X1Z0
A	514	TRP	-	expression tag	UNP H6X1Z0
A	515	VAL	-	expression tag	UNP H6X1Z0
A	516	LEU	-	expression tag	UNP H6X1Z0
A	517	LEU	-	expression tag	UNP H6X1Z0
A	518	SER	-	expression tag	UNP H6X1Z0
A	519	THR	-	expression tag	UNP H6X1Z0
A	520	PHE	-	expression tag	UNP H6X1Z0
A	521	LEU	-	expression tag	UNP H6X1Z0
A	522	GLY	-	expression tag	UNP H6X1Z0
A	523	ARG	-	expression tag	UNP H6X1Z0
A	524	SER	-	expression tag	UNP H6X1Z0
A	525	LEU	-	expression tag	UNP H6X1Z0
A	526	GLU	-	expression tag	UNP H6X1Z0
A	527	VAL	-	expression tag	UNP H6X1Z0
A	528	LEU	-	expression tag	UNP H6X1Z0
A	529	PHE	-	expression tag	UNP H6X1Z0
A	530	GLN	-	expression tag	UNP H6X1Z0
A	531	GLY	-	expression tag	UNP H6X1Z0
A	532	PRO	-	expression tag	UNP H6X1Z0
A	533	GLY	-	expression tag	UNP H6X1Z0
A	534	HIS	-	expression tag	UNP H6X1Z0
A	535	HIS	-	expression tag	UNP H6X1Z0
A	536	HIS	-	expression tag	UNP H6X1Z0
A	537	HIS	-	expression tag	UNP H6X1Z0
A	538	HIS	-	expression tag	UNP H6X1Z0
A	539	HIS	-	expression tag	UNP H6X1Z0
A	540	HIS	-	expression tag	UNP H6X1Z0
A	541	HIS	-	expression tag	UNP H6X1Z0
A	542	SER	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	543	ALA	-	expression tag	UNP H6X1Z0
A	544	TRP	-	expression tag	UNP H6X1Z0
A	545	SER	-	expression tag	UNP H6X1Z0
A	546	HIS	-	expression tag	UNP H6X1Z0
A	547	PRO	-	expression tag	UNP H6X1Z0
A	548	GLN	-	expression tag	UNP H6X1Z0
A	549	PHE	-	expression tag	UNP H6X1Z0
A	550	GLU	-	expression tag	UNP H6X1Z0
A	551	LYS	-	expression tag	UNP H6X1Z0
E	100	ARG	GLN	engineered mutation	UNP H6X1Z0
E	101	ARG	SER	engineered mutation	UNP H6X1Z0
E	110	CYS	LEU	engineered mutation	UNP H6X1Z0
E	127	CYS	THR	engineered mutation	UNP H6X1Z0
E	140	CYS	ALA	engineered mutation	UNP H6X1Z0
E	147	CYS	ALA	engineered mutation	UNP H6X1Z0
E	153	CYS	ASN	engineered mutation	UNP H6X1Z0
E	185	PRO	ALA	engineered mutation	UNP H6X1Z0
E	219	LYS	LEU	engineered mutation	UNP H6X1Z0
E	231	ILE	VAL	engineered mutation	UNP H6X1Z0
E	322	CYS	ASN	engineered mutation	UNP H6X1Z0
E	365	CYS	THR	engineered mutation	UNP H6X1Z0
E	453	GLN	GLU	engineered mutation	UNP H6X1Z0
E	463	CYS	VAL	engineered mutation	UNP H6X1Z0
E	491	GLY	-	expression tag	UNP H6X1Z0
E	492	GLY	-	expression tag	UNP H6X1Z0
E	493	GLY	-	expression tag	UNP H6X1Z0
E	494	SER	-	expression tag	UNP H6X1Z0
E	495	GLY	-	expression tag	UNP H6X1Z0
E	496	TYR	-	expression tag	UNP H6X1Z0
E	497	ILE	-	expression tag	UNP H6X1Z0
E	498	PRO	-	expression tag	UNP H6X1Z0
E	499	GLU	-	expression tag	UNP H6X1Z0
E	500	ALA	-	expression tag	UNP H6X1Z0
E	501	PRO	-	expression tag	UNP H6X1Z0
E	502	ARG	-	expression tag	UNP H6X1Z0
E	503	ASP	-	expression tag	UNP H6X1Z0
E	504	GLY	-	expression tag	UNP H6X1Z0
E	505	GLN	-	expression tag	UNP H6X1Z0
E	506	ALA	-	expression tag	UNP H6X1Z0
E	507	TYR	-	expression tag	UNP H6X1Z0
E	508	VAL	-	expression tag	UNP H6X1Z0
E	509	ARG	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	510	LYS	-	expression tag	UNP H6X1Z0
E	511	ASP	-	expression tag	UNP H6X1Z0
E	512	GLY	-	expression tag	UNP H6X1Z0
E	513	GLU	-	expression tag	UNP H6X1Z0
E	514	TRP	-	expression tag	UNP H6X1Z0
E	515	VAL	-	expression tag	UNP H6X1Z0
E	516	LEU	-	expression tag	UNP H6X1Z0
E	517	LEU	-	expression tag	UNP H6X1Z0
E	518	SER	-	expression tag	UNP H6X1Z0
E	519	THR	-	expression tag	UNP H6X1Z0
E	520	PHE	-	expression tag	UNP H6X1Z0
E	521	LEU	-	expression tag	UNP H6X1Z0
E	522	GLY	-	expression tag	UNP H6X1Z0
E	523	ARG	-	expression tag	UNP H6X1Z0
E	524	SER	-	expression tag	UNP H6X1Z0
E	525	LEU	-	expression tag	UNP H6X1Z0
E	526	GLU	-	expression tag	UNP H6X1Z0
E	527	VAL	-	expression tag	UNP H6X1Z0
E	528	LEU	-	expression tag	UNP H6X1Z0
E	529	PHE	-	expression tag	UNP H6X1Z0
E	530	GLN	-	expression tag	UNP H6X1Z0
E	531	GLY	-	expression tag	UNP H6X1Z0
E	532	PRO	-	expression tag	UNP H6X1Z0
E	533	GLY	-	expression tag	UNP H6X1Z0
E	534	HIS	-	expression tag	UNP H6X1Z0
E	535	HIS	-	expression tag	UNP H6X1Z0
E	536	HIS	-	expression tag	UNP H6X1Z0
E	537	HIS	-	expression tag	UNP H6X1Z0
E	538	HIS	-	expression tag	UNP H6X1Z0
E	539	HIS	-	expression tag	UNP H6X1Z0
E	540	HIS	-	expression tag	UNP H6X1Z0
E	541	HIS	-	expression tag	UNP H6X1Z0
E	542	SER	-	expression tag	UNP H6X1Z0
E	543	ALA	-	expression tag	UNP H6X1Z0
E	544	TRP	-	expression tag	UNP H6X1Z0
E	545	SER	-	expression tag	UNP H6X1Z0
E	546	HIS	-	expression tag	UNP H6X1Z0
E	547	PRO	-	expression tag	UNP H6X1Z0
E	548	GLN	-	expression tag	UNP H6X1Z0
E	549	PHE	-	expression tag	UNP H6X1Z0
E	550	GLU	-	expression tag	UNP H6X1Z0
E	551	LYS	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	100	ARG	GLN	engineered mutation	UNP H6X1Z0
F	101	ARG	SER	engineered mutation	UNP H6X1Z0
F	110	CYS	LEU	engineered mutation	UNP H6X1Z0
F	127	CYS	THR	engineered mutation	UNP H6X1Z0
F	140	CYS	ALA	engineered mutation	UNP H6X1Z0
F	147	CYS	ALA	engineered mutation	UNP H6X1Z0
F	153	CYS	ASN	engineered mutation	UNP H6X1Z0
F	185	PRO	ALA	engineered mutation	UNP H6X1Z0
F	219	LYS	LEU	engineered mutation	UNP H6X1Z0
F	231	ILE	VAL	engineered mutation	UNP H6X1Z0
F	322	CYS	ASN	engineered mutation	UNP H6X1Z0
F	365	CYS	THR	engineered mutation	UNP H6X1Z0
F	453	GLN	GLU	engineered mutation	UNP H6X1Z0
F	463	CYS	VAL	engineered mutation	UNP H6X1Z0
F	491	GLY	-	expression tag	UNP H6X1Z0
F	492	GLY	-	expression tag	UNP H6X1Z0
F	493	GLY	-	expression tag	UNP H6X1Z0
F	494	SER	-	expression tag	UNP H6X1Z0
F	495	GLY	-	expression tag	UNP H6X1Z0
F	496	TYR	-	expression tag	UNP H6X1Z0
F	497	ILE	-	expression tag	UNP H6X1Z0
F	498	PRO	-	expression tag	UNP H6X1Z0
F	499	GLU	-	expression tag	UNP H6X1Z0
F	500	ALA	-	expression tag	UNP H6X1Z0
F	501	PRO	-	expression tag	UNP H6X1Z0
F	502	ARG	-	expression tag	UNP H6X1Z0
F	503	ASP	-	expression tag	UNP H6X1Z0
F	504	GLY	-	expression tag	UNP H6X1Z0
F	505	GLN	-	expression tag	UNP H6X1Z0
F	506	ALA	-	expression tag	UNP H6X1Z0
F	507	TYR	-	expression tag	UNP H6X1Z0
F	508	VAL	-	expression tag	UNP H6X1Z0
F	509	ARG	-	expression tag	UNP H6X1Z0
F	510	LYS	-	expression tag	UNP H6X1Z0
F	511	ASP	-	expression tag	UNP H6X1Z0
F	512	GLY	-	expression tag	UNP H6X1Z0
F	513	GLU	-	expression tag	UNP H6X1Z0
F	514	TRP	-	expression tag	UNP H6X1Z0
F	515	VAL	-	expression tag	UNP H6X1Z0
F	516	LEU	-	expression tag	UNP H6X1Z0
F	517	LEU	-	expression tag	UNP H6X1Z0
F	518	SER	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	519	THR	-	expression tag	UNP H6X1Z0
F	520	PHE	-	expression tag	UNP H6X1Z0
F	521	LEU	-	expression tag	UNP H6X1Z0
F	522	GLY	-	expression tag	UNP H6X1Z0
F	523	ARG	-	expression tag	UNP H6X1Z0
F	524	SER	-	expression tag	UNP H6X1Z0
F	525	LEU	-	expression tag	UNP H6X1Z0
F	526	GLU	-	expression tag	UNP H6X1Z0
F	527	VAL	-	expression tag	UNP H6X1Z0
F	528	LEU	-	expression tag	UNP H6X1Z0
F	529	PHE	-	expression tag	UNP H6X1Z0
F	530	GLN	-	expression tag	UNP H6X1Z0
F	531	GLY	-	expression tag	UNP H6X1Z0
F	532	PRO	-	expression tag	UNP H6X1Z0
F	533	GLY	-	expression tag	UNP H6X1Z0
F	534	HIS	-	expression tag	UNP H6X1Z0
F	535	HIS	-	expression tag	UNP H6X1Z0
F	536	HIS	-	expression tag	UNP H6X1Z0
F	537	HIS	-	expression tag	UNP H6X1Z0
F	538	HIS	-	expression tag	UNP H6X1Z0
F	539	HIS	-	expression tag	UNP H6X1Z0
F	540	HIS	-	expression tag	UNP H6X1Z0
F	541	HIS	-	expression tag	UNP H6X1Z0
F	542	SER	-	expression tag	UNP H6X1Z0
F	543	ALA	-	expression tag	UNP H6X1Z0
F	544	TRP	-	expression tag	UNP H6X1Z0
F	545	SER	-	expression tag	UNP H6X1Z0
F	546	HIS	-	expression tag	UNP H6X1Z0
F	547	PRO	-	expression tag	UNP H6X1Z0
F	548	GLN	-	expression tag	UNP H6X1Z0
F	549	PHE	-	expression tag	UNP H6X1Z0
F	550	GLU	-	expression tag	UNP H6X1Z0
F	551	LYS	-	expression tag	UNP H6X1Z0

- Molecule 2 is a protein called MPE8 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			786	486	135	163	2		
2	M	107	Total	C	N	O	S	0	0
			786	486	135	163	2		
2	O	107	Total	C	N	O	S	0	0
			786	486	135	163	2		



- Molecule 3 is a protein called ADI-61026 heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	121	Total	C	N	O	S	1	0
			963	618	157	182	6		
3	H	121	Total	C	N	O	S	1	0
			963	618	157	182	6		
3	I	121	Total	C	N	O	S	1	0
			963	618	157	182	6		

- Molecule 4 is a protein called ADI-61026 light.

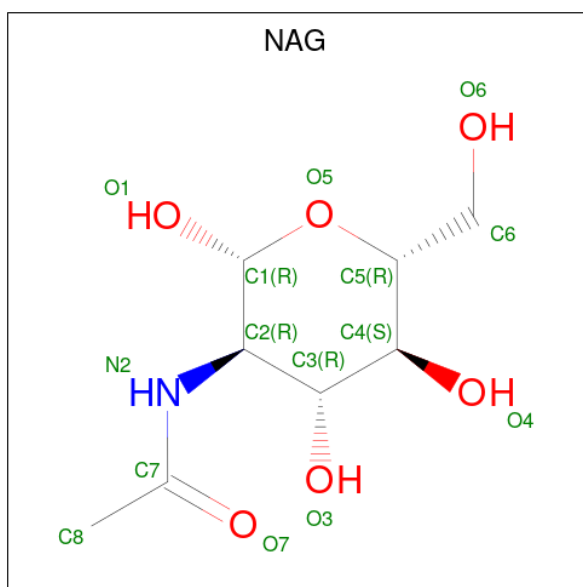
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	106	Total	C	N	O	S	0	0
			797	499	130	164	4		
4	K	106	Total	C	N	O	S	0	0
			797	499	130	164	4		
4	L	106	Total	C	N	O	S	0	0
			797	499	130	164	4		

- Molecule 5 is a protein called MPE8 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	122	Total	C	N	O	S	0	0
			923	581	157	181	4		
5	J	122	Total	C	N	O	S	0	0
			923	581	157	181	4		
5	N	122	Total	C	N	O	S	0	0
			923	581	157	181	4		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





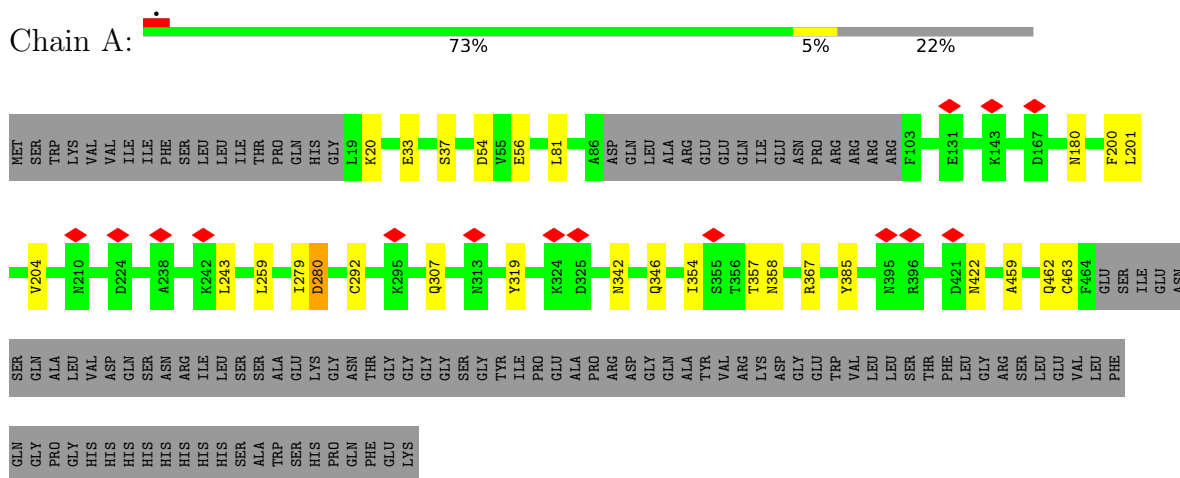
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	1	5	0
6	E	1	14	8	1	5	0
6	F	1	14	8	1	5	0



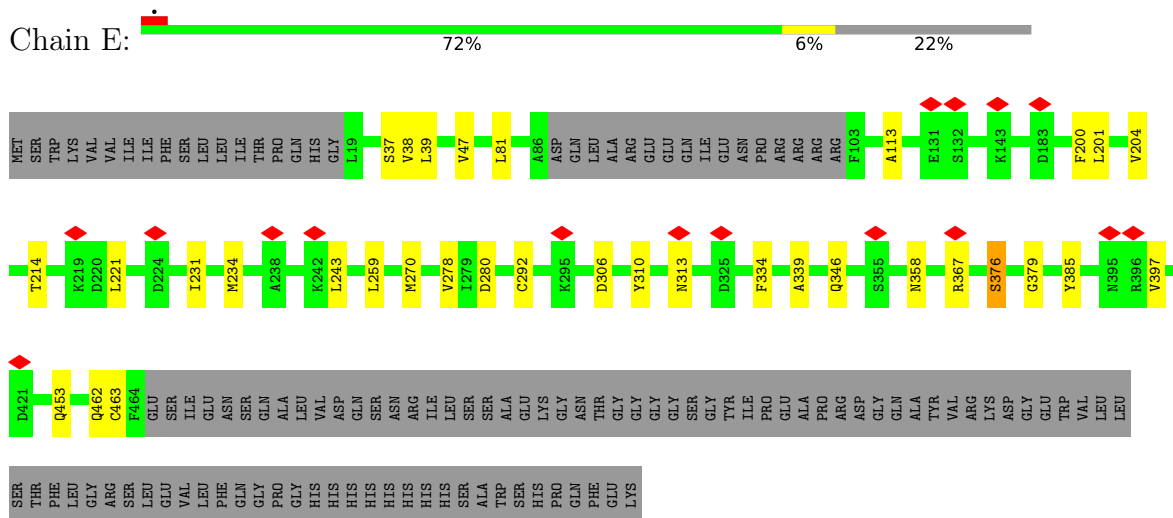
### 3 Residue-property plots

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: Fusion glycoprotein F0



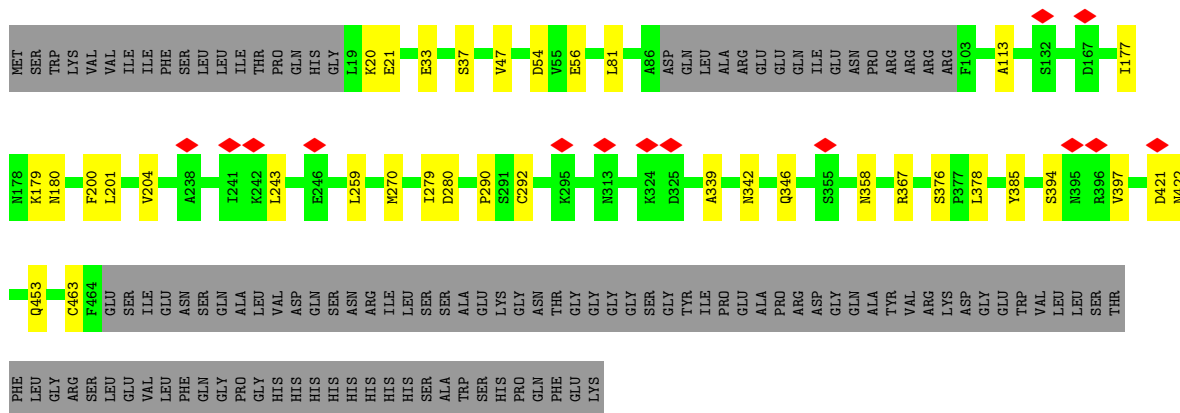
#### • Molecule 1: Fusion glycoprotein F0



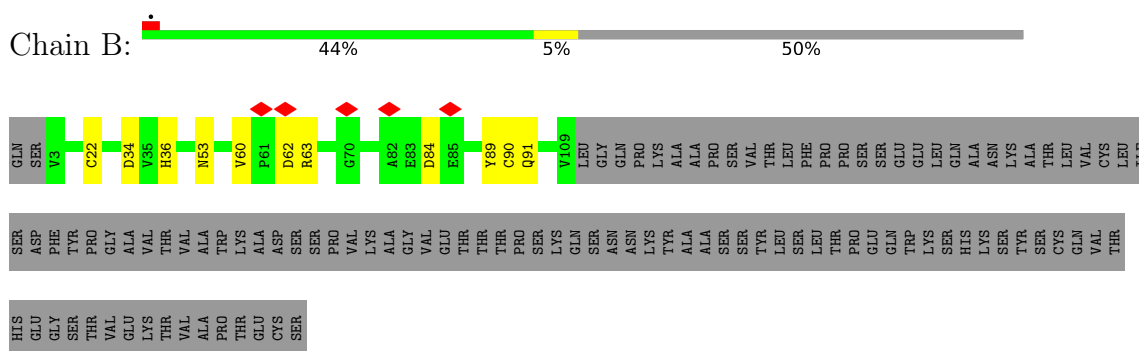
#### • Molecule 1: Fusion glycoprotein F0



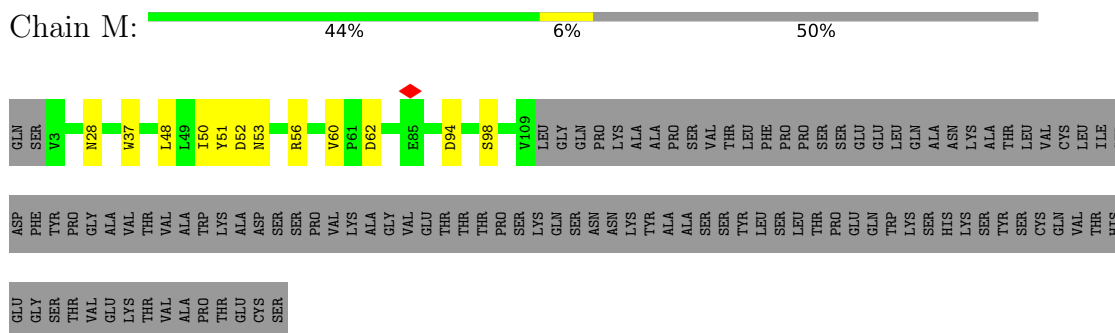




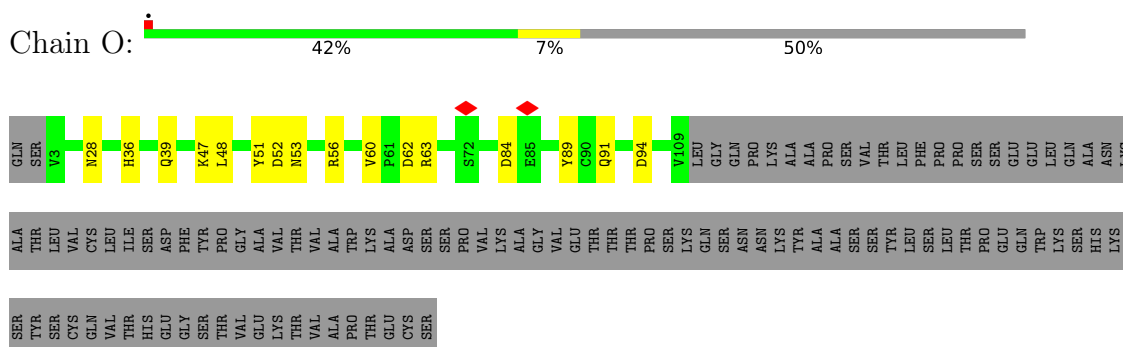
- Molecule 2: MPE8 light chain



- Molecule 2: MPE8 light chain



- Molecule 2: MPE8 light chain







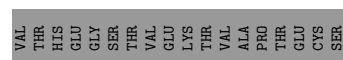




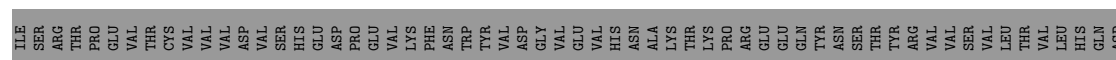
Chain K:  16% 46% 50%



Chain L:  45% 50%



Chain G:  23% 73%









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113336	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 ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	74.062	Depositor
Minimum map value	-3.725	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.019	Depositor
Recommended contour level	6.2	Depositor
Map size ( $\text{\AA}$ )	349.92, 349.92, 349.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.366875, 1.366875, 1.366875	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	A	0.25	0/3308	0.51	0/4479
1	E	0.25	0/3308	0.51	0/4479
1	F	0.25	0/3308	0.52	0/4479
2	B	0.24	0/803	0.51	0/1096
2	M	0.26	0/803	0.53	0/1096
2	O	0.25	0/803	0.53	0/1096
3	C	0.23	0/980	0.54	0/1338
3	H	0.23	0/980	0.52	0/1338
3	I	0.23	0/980	0.54	0/1338
4	D	0.25	0/814	0.53	0/1105
4	K	0.24	0/814	0.53	0/1105
4	L	0.25	0/814	0.53	0/1105
5	G	0.24	0/943	0.55	0/1276
5	J	0.24	0/943	0.51	0/1276
5	N	0.25	0/943	0.53	0/1276
All	All	0.25	0/20544	0.52	0/27882

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3260	0	3273	20	0
1	E	3260	0	3273	17	0
1	F	3260	0	3273	26	0
2	B	786	0	749	5	0
2	M	786	0	749	7	0
2	O	786	0	749	8	0
3	C	963	0	949	12	0
3	H	963	0	949	8	0
3	I	963	0	949	10	0
4	D	797	0	769	4	0
4	K	797	0	769	3	0
4	L	797	0	769	5	0
5	G	923	0	893	9	0
5	J	923	0	893	6	0
5	N	923	0	893	6	0
6	A	14	0	13	1	0
6	E	14	0	13	0	0
6	F	14	0	13	1	0
All	All	20229	0	19938	125	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 3.

The worst 5 of 125 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:F:422:ASN:OD1	5:G:100:ARG:NH2	2.21	0.69
2:M:60:VAL:HG12	2:M:62:ASP:H	1.61	0.66
2:O:60:VAL:HG12	2:O:62:ASP:H	1.65	0.62
1:A:54:ASP:OD2	3:C:100(A):LYS:NZ	2.30	0.60
2:O:56:ARG:NH1	2:O:62:ASP:OD1	2.34	0.60

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/551 (77%)	398 (93%)	28 (7%)	0	100	100
1	E	426/551 (77%)	405 (95%)	21 (5%)	0	100	100
1	F	426/551 (77%)	398 (93%)	28 (7%)	0	100	100
2	B	105/216 (49%)	100 (95%)	5 (5%)	0	100	100
2	M	105/216 (49%)	98 (93%)	7 (7%)	0	100	100
2	O	105/216 (49%)	99 (94%)	6 (6%)	0	100	100
3	C	119/228 (52%)	111 (93%)	7 (6%)	1 (1%)	19	57
3	H	119/228 (52%)	116 (98%)	2 (2%)	1 (1%)	19	57
3	I	119/228 (52%)	112 (94%)	6 (5%)	1 (1%)	19	57
4	D	104/214 (49%)	100 (96%)	4 (4%)	0	100	100
4	K	104/214 (49%)	100 (96%)	4 (4%)	0	100	100
4	L	104/214 (49%)	98 (94%)	6 (6%)	0	100	100
5	G	120/454 (26%)	112 (93%)	8 (7%)	0	100	100
5	J	120/454 (26%)	109 (91%)	11 (9%)	0	100	100
5	N	120/454 (26%)	113 (94%)	7 (6%)	0	100	100
All	All	2622/4989 (53%)	2469 (94%)	150 (6%)	3 (0%)	54	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	100	TRP
3	C	100	TRP
3	H	100	TRP

### 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	365/468 (78%)	363 (100%)	2 (0%)	88	95

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	365/468 (78%)	360 (99%)	5 (1%)	67	85
1	F	365/468 (78%)	362 (99%)	3 (1%)	81	92
2	B	87/181 (48%)	84 (97%)	3 (3%)	37	67
2	M	87/181 (48%)	87 (100%)	0	100	100
2	O	87/181 (48%)	86 (99%)	1 (1%)	73	88
3	C	108/202 (54%)	107 (99%)	1 (1%)	78	91
3	H	108/202 (54%)	107 (99%)	1 (1%)	78	91
3	I	108/202 (54%)	107 (99%)	1 (1%)	78	91
4	D	89/182 (49%)	86 (97%)	3 (3%)	37	67
4	K	89/182 (49%)	85 (96%)	4 (4%)	27	60
4	L	89/182 (49%)	86 (97%)	3 (3%)	37	67
5	G	98/399 (25%)	97 (99%)	1 (1%)	76	89
5	J	98/399 (25%)	97 (99%)	1 (1%)	76	89
5	N	98/399 (25%)	96 (98%)	2 (2%)	55	79
All	All	2241/4296 (52%)	2210 (99%)	31 (1%)	68	85

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	342	ASN
4	L	107	LEU
5	G	108	THR
5	N	108	THR
4	K	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
5	G	35	ASN
3	H	16	GLN
2	M	28	ASN
2	O	28	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

3 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	A	601	1	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
6	NAG	F	601	1	14,14,15	0.72	0	17,19,21	0.56	0
6	NAG	E	601	1	14,14,15	0.43	0	17,19,21	0.78	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	A	601	1	-	0/6/23/26	0/1/1/1
6	NAG	F	601	1	-	0/6/23/26	0/1/1/1
6	NAG	E	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	A	601	NAG	C1-O5-C5	2.17	115.13	112.19
6	E	601	NAG	C1-O5-C5	2.11	115.06	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	NAG	1	0
6	F	601	NAG	1	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.



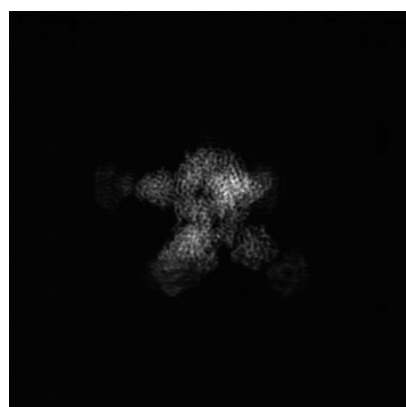
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27024. These allow visual inspection of the internal detail of the map and identification of artifacts.

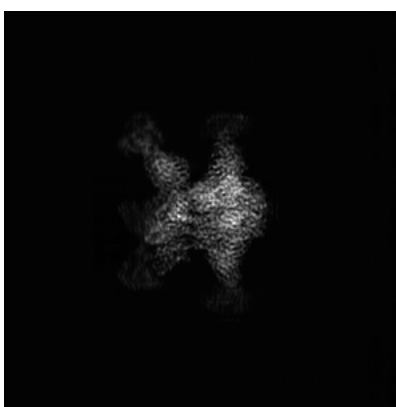
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

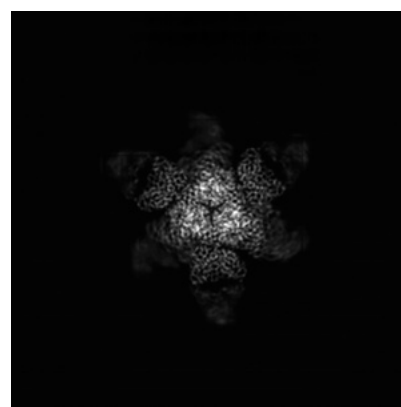
#### 6.1.1 Primary map



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: 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: 122



Y Index: 118



Z Index: 146

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation

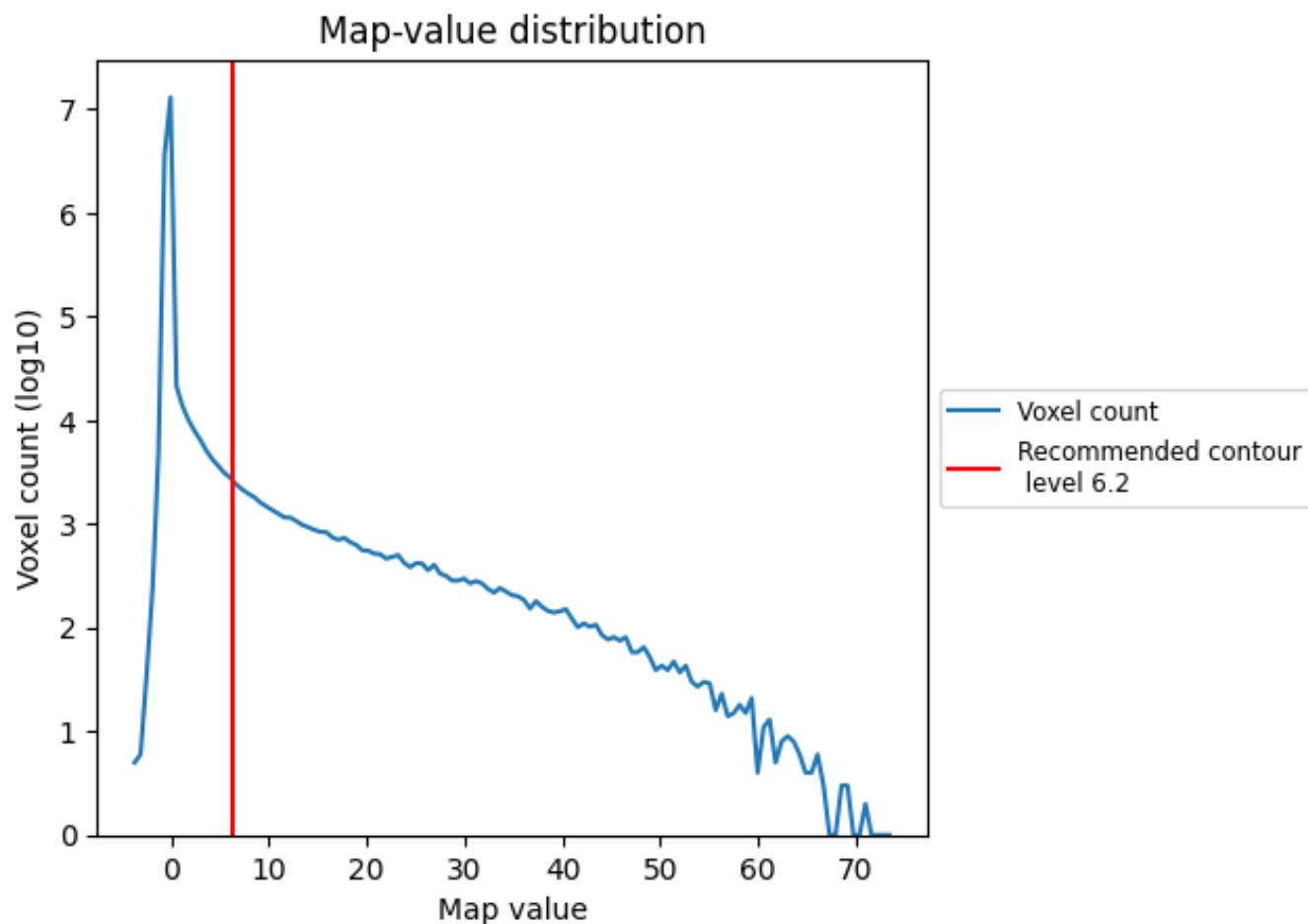
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

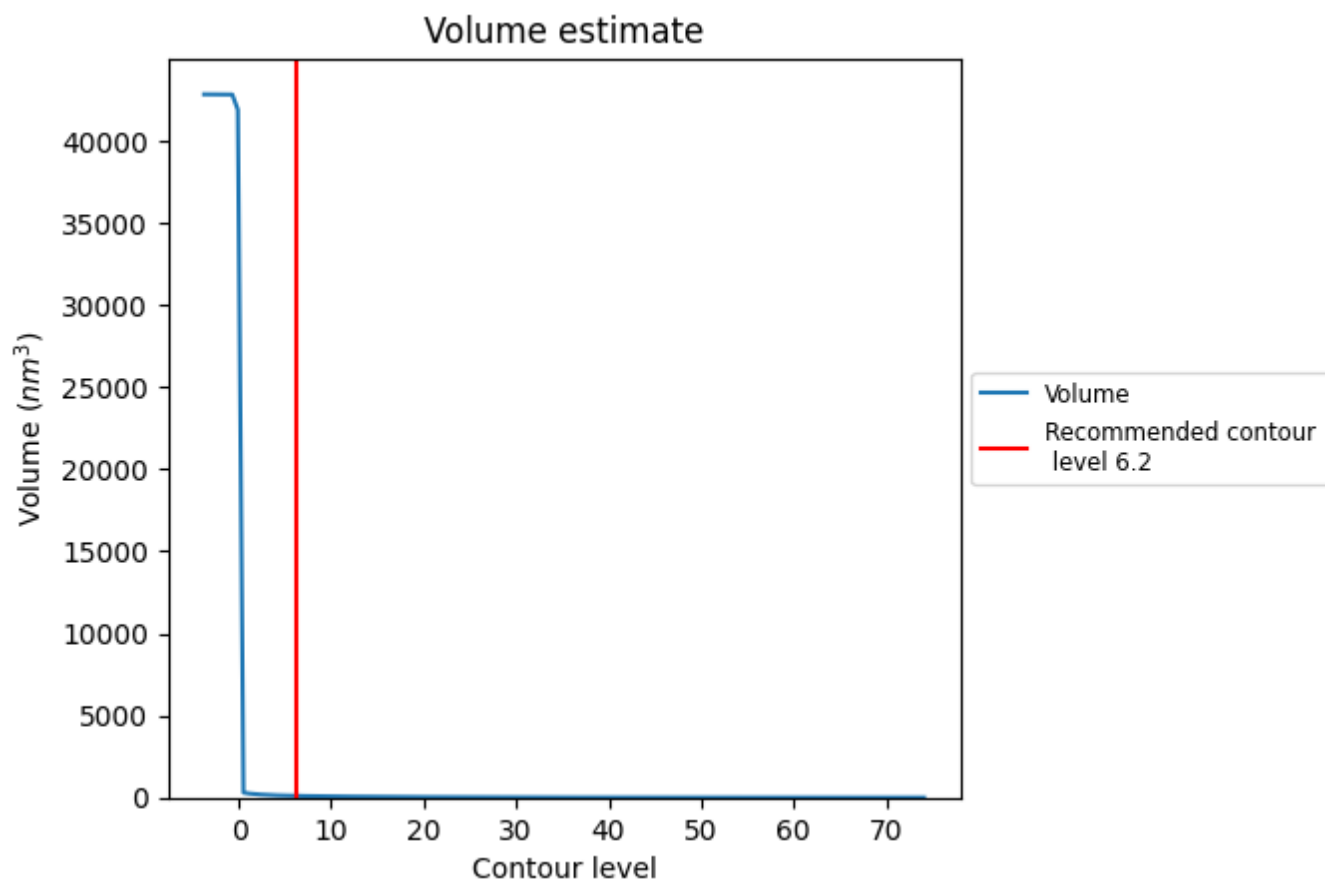
### 7.1 Map-value distribution [i](#)



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](#)

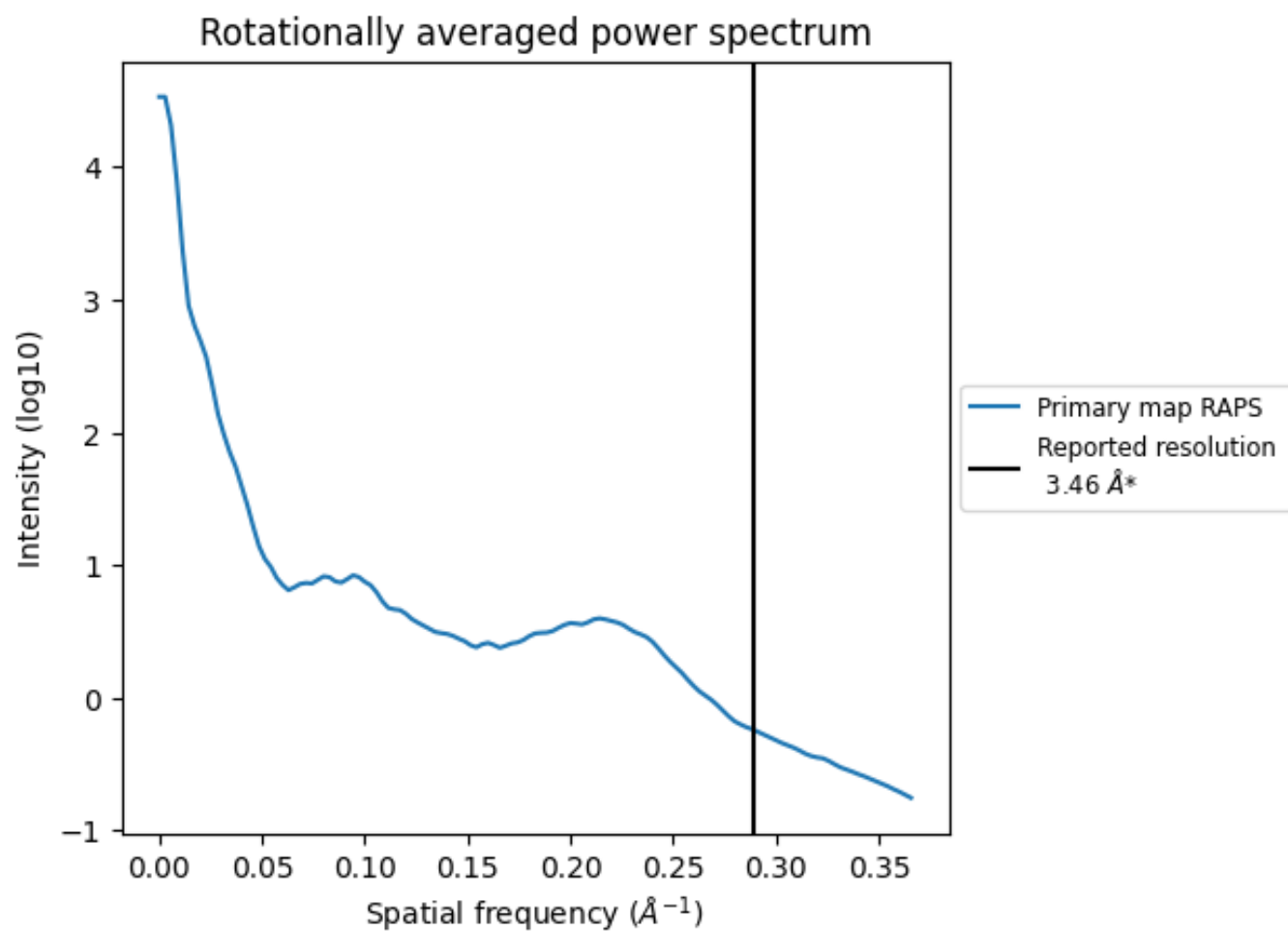


The volume at the recommended contour level is 103  $\text{nm}^3$ ; this corresponds to an approximate mass of 93 kDa.

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 0.289 Å<sup>-1</sup>



## 8 Fourier-Shell correlation ⓘ

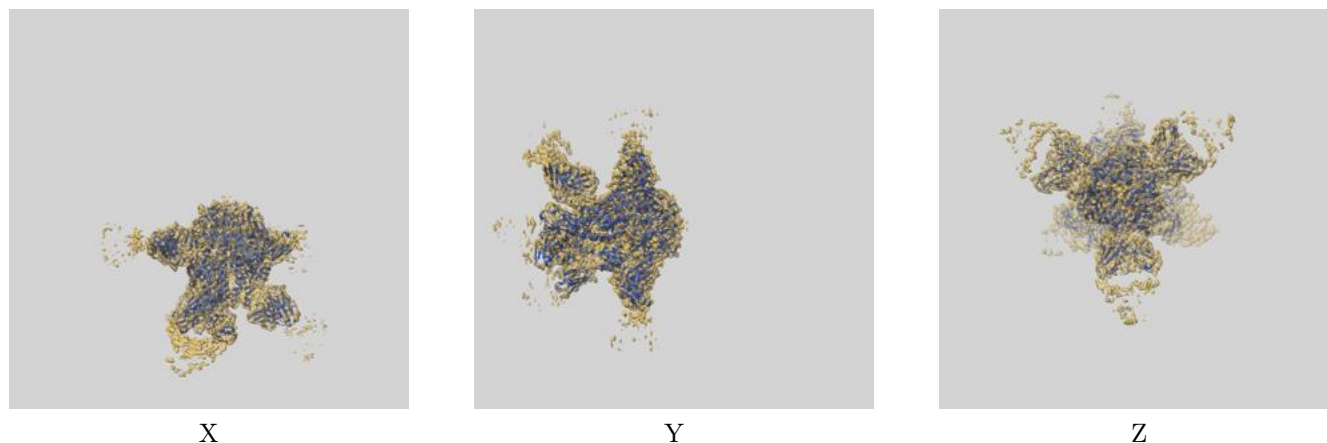
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27024 and PDB model 8CW9. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

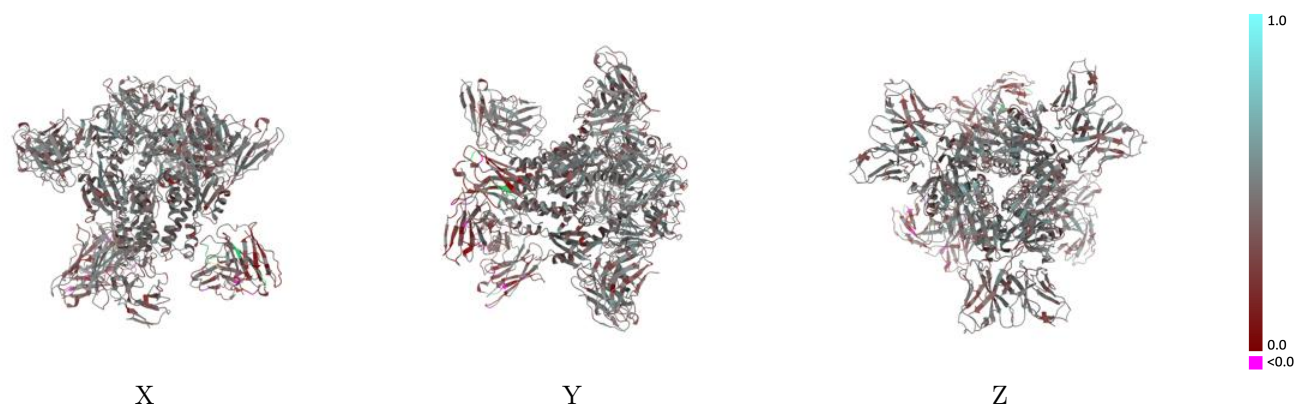
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 6.2 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.

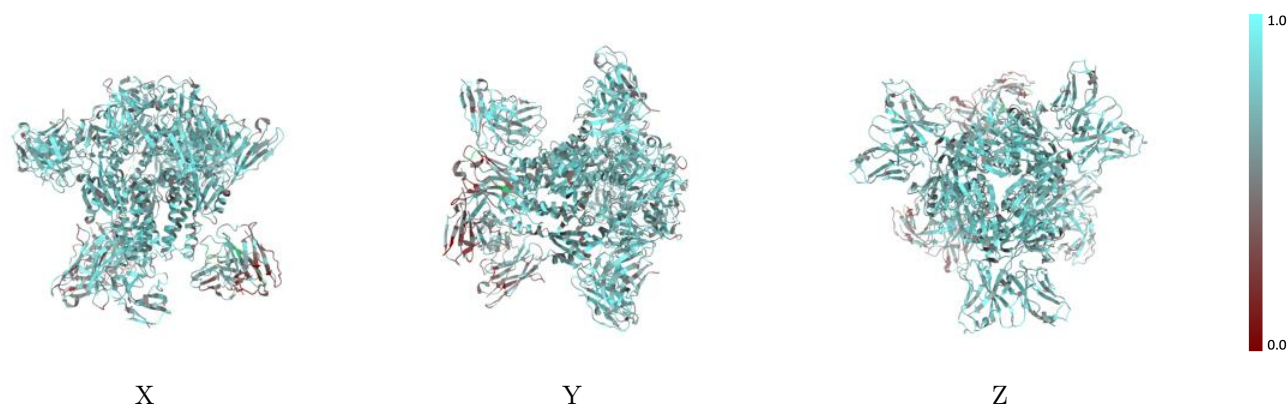


## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according 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.

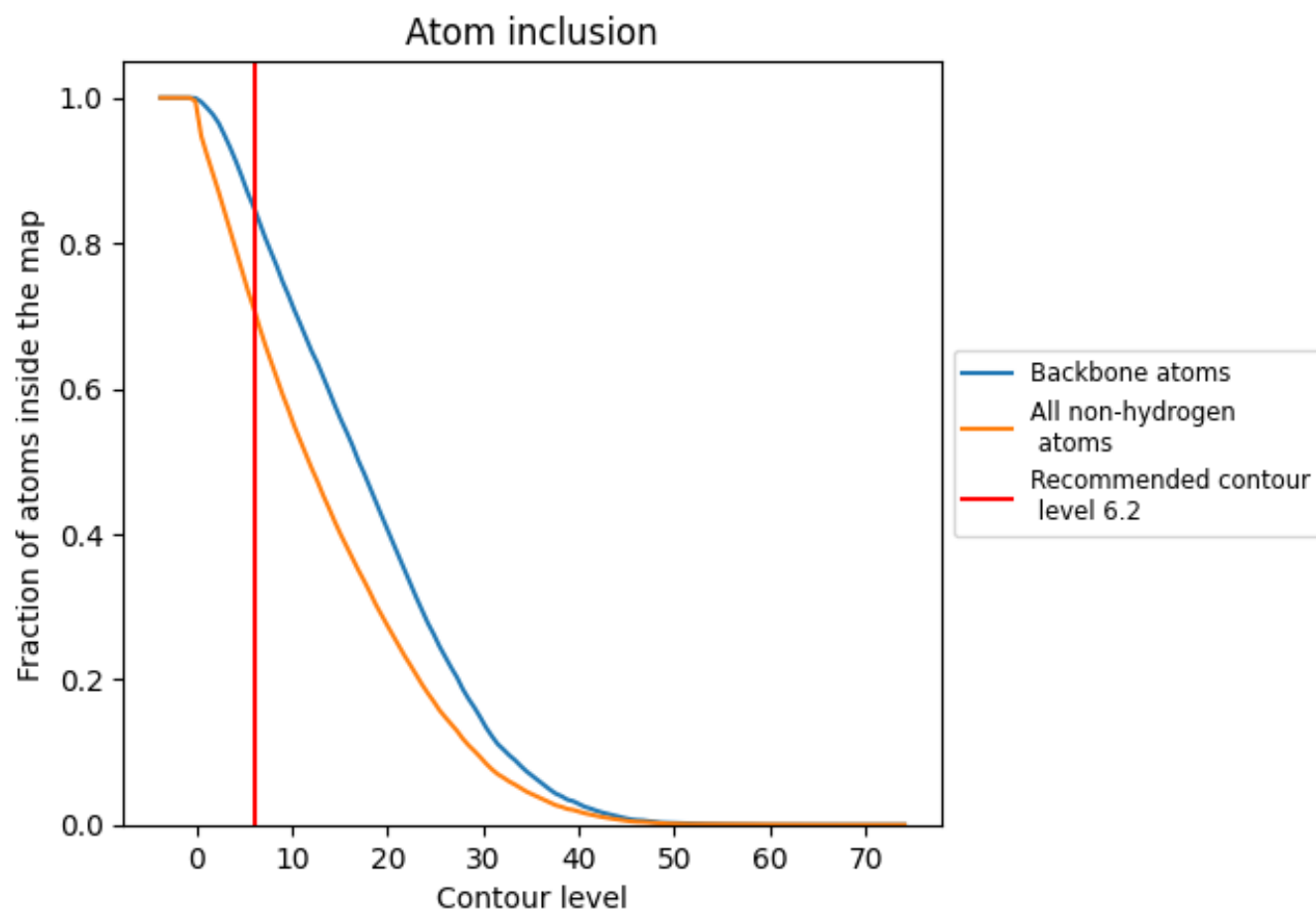
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (6.2).



## 9.4 Atom inclusion [i](#)



































At the recommended contour level, 84% of all backbone atoms, 70% 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 (6.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7029	 0.4190
A	 0.7360	 0.4490
B	 0.7237	 0.4320
C	 0.5486	 0.3140
D	 0.5478	 0.3040
E	 0.7373	 0.4470
F	 0.7488	 0.4530
G	 0.7222	 0.4280
H	 0.7150	 0.4320
I	 0.5656	 0.3250
J	 0.7422	 0.4350
K	 0.5172	 0.3100
L	 0.7045	 0.3980
M	 0.7393	 0.4400
N	 0.7511	 0.4330
O	 0.7315	 0.4320

