



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 12:39 AM EDT

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

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

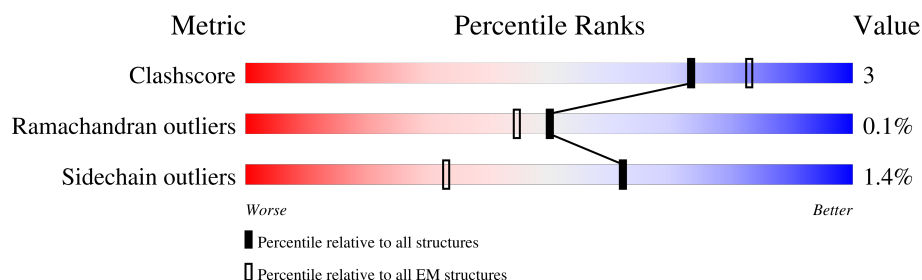
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



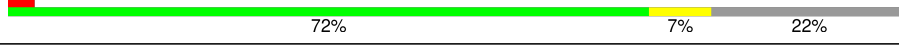
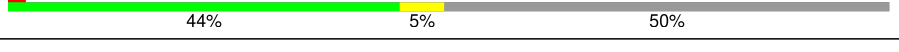
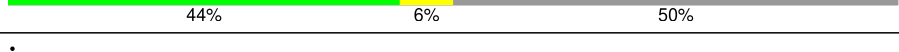
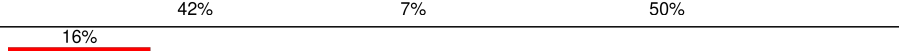
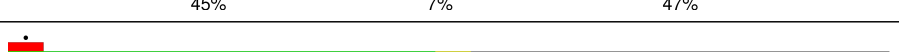
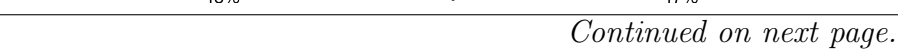
The reported resolution of this entry is 3.46 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	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>16%45%8%47%</div></div>
4	D	214	<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>16%46%.50%</div></div>
4	L	214	<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>.23%.73%</div></div>
5	J	454	<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>.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		

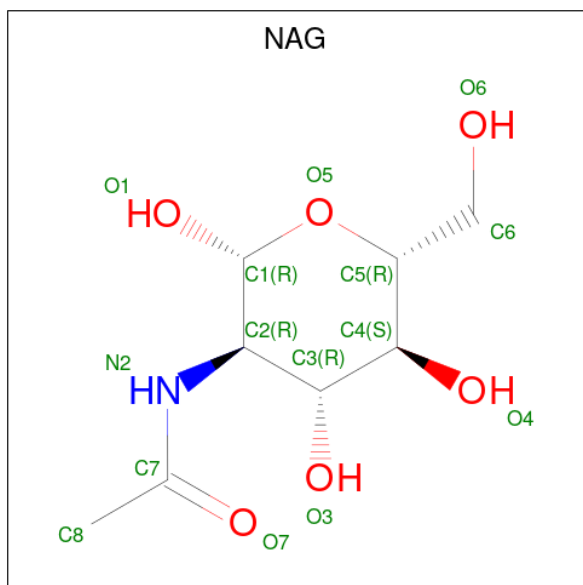
- Molecule 4 is a protein called ADI-61026 light.

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: C₈H₁₅NO₆).

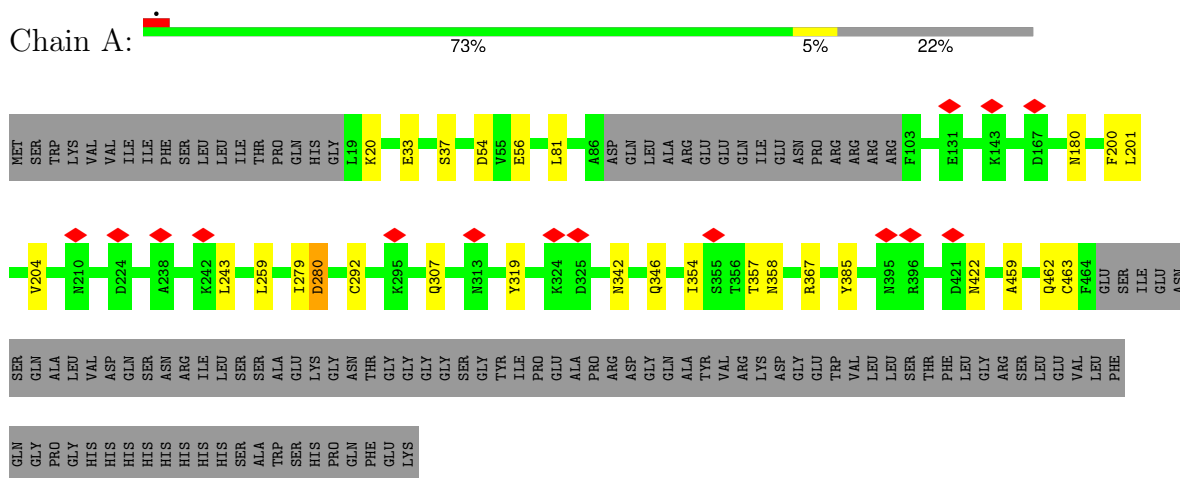


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	

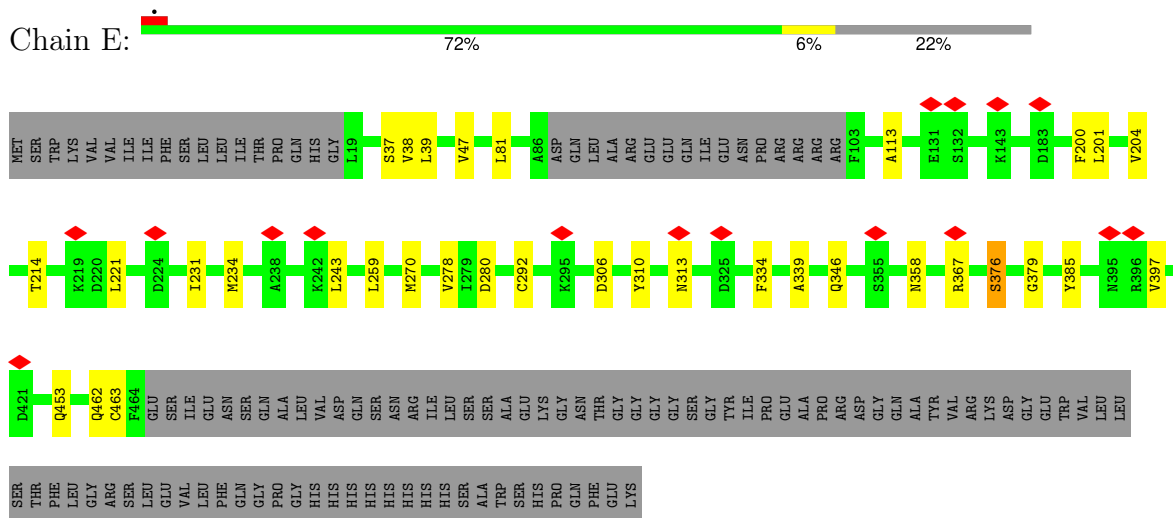
3 Residue-property plots

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: Fusion glycoprotein F0

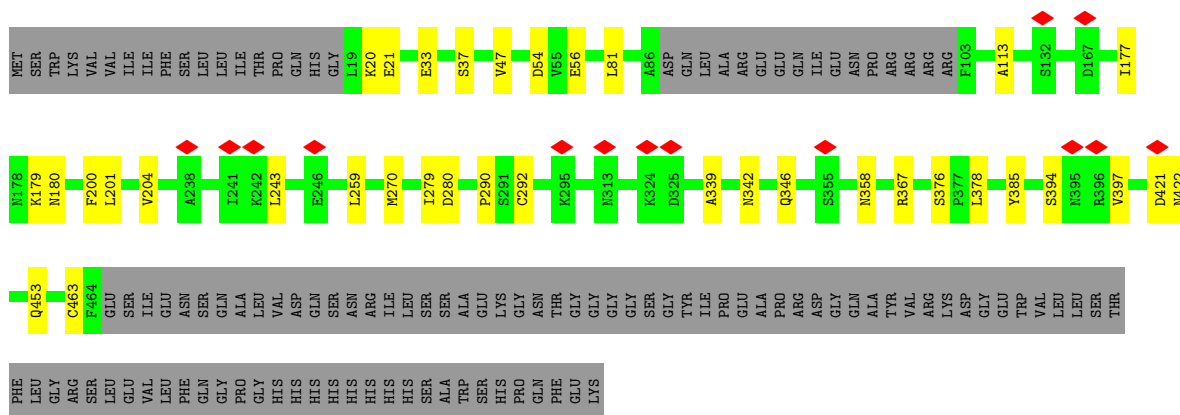


• Molecule 1: Fusion glycoprotein F0

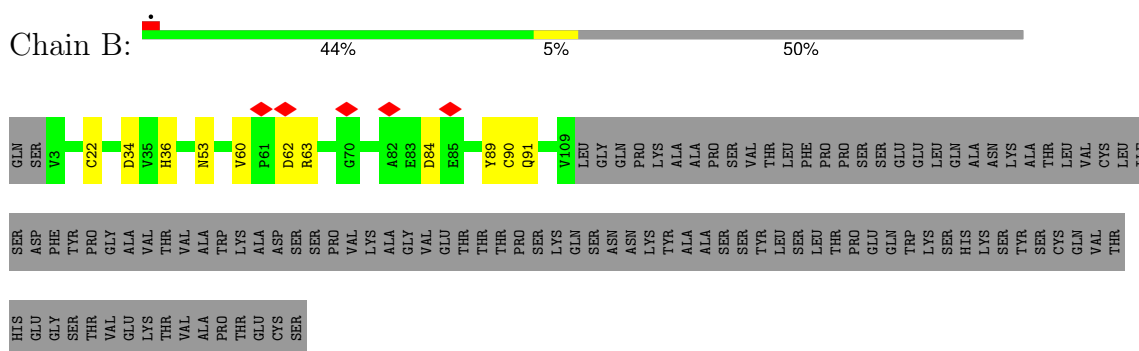


• Molecule 1: Fusion glycoprotein F0

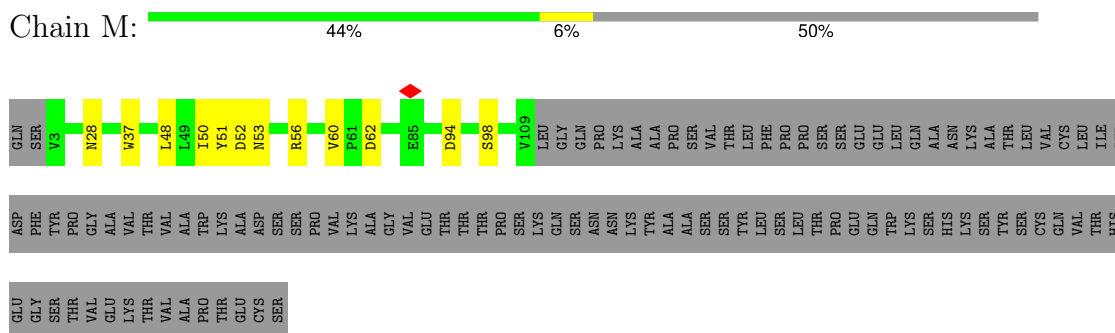




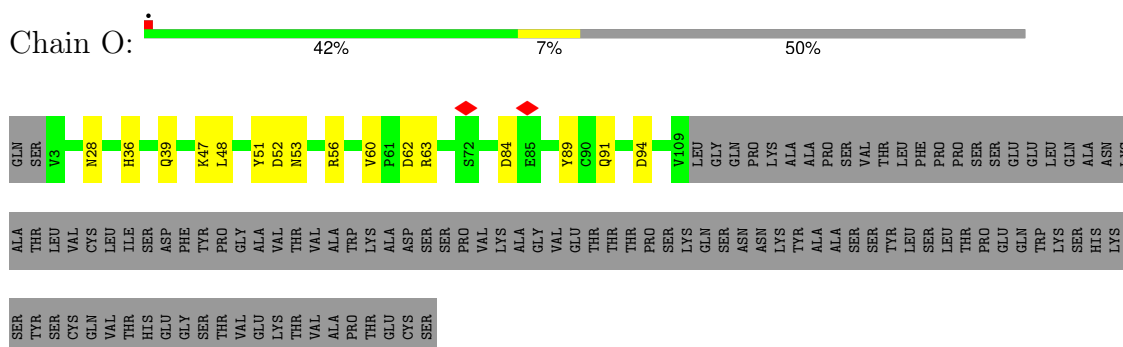
- Molecule 2: MPE8 light chain



- Molecule 2: MPE8 light chain



- Molecule 2: MPE8 light chain



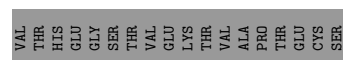




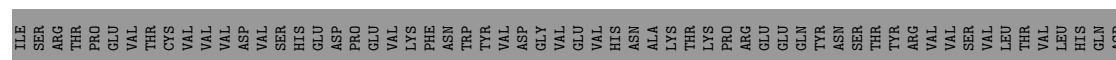
Chain K:  16% 46% 50%



Chain L: 

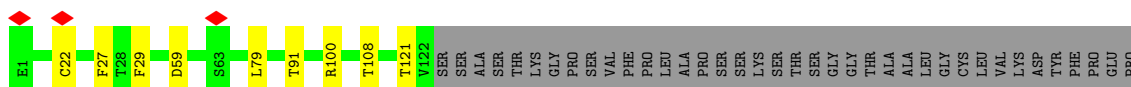


Chain G:  23% 73%



HIS	ASN	HIS	TYR	THR	GLN	LYS	SER	LEU	SER	LEU	SER	PRO	GLY	LYS
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- Molecule 5: MPE8 heavy chain



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

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

THR	PRO	PRO	VAL	LEU	ASP	SER	ASP	GLY	SER	PHE	PHE	LEU	TYR	SER	LYS	LEU	THR	VAL	ASP	LYS	SER	ARG	TRP	GLN	GLN	GLY	ASN	VAL	PHE	SER	CYS	SER	VAL	MET	HIS	GLU	HIS	ALA	LEU	ASN	HIS	HIS	TYR	THR	GLN	LYS	SER	LEU	SER	PRO	GLY	LYS
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- Molecule 5: MPE8 heavy chain



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

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

SER
PRO
GLY
LYS

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 (\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 (\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%)	16	50
3	H	119/228 (52%)	116 (98%)	2 (2%)	1 (1%)	16	50
3	I	119/228 (52%)	112 (94%)	6 (5%)	1 (1%)	16	50
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%)	50	79

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%)	86	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	365/468 (78%)	360 (99%)	5 (1%)	62	79
1	F	365/468 (78%)	362 (99%)	3 (1%)	79	87
2	B	87/181 (48%)	84 (97%)	3 (3%)	32	61
2	M	87/181 (48%)	87 (100%)	0	100	100
2	O	87/181 (48%)	86 (99%)	1 (1%)	70	83
3	C	108/202 (54%)	107 (99%)	1 (1%)	75	86
3	H	108/202 (54%)	107 (99%)	1 (1%)	75	86
3	I	108/202 (54%)	107 (99%)	1 (1%)	75	86
4	D	89/182 (49%)	86 (97%)	3 (3%)	32	61
4	K	89/182 (49%)	85 (96%)	4 (4%)	23	54
4	L	89/182 (49%)	86 (97%)	3 (3%)	32	61
5	G	98/399 (25%)	97 (99%)	1 (1%)	73	84
5	J	98/399 (25%)	97 (99%)	1 (1%)	73	84
5	N	98/399 (25%)	96 (98%)	2 (2%)	50	73
All	All	2241/4296 (52%)	2210 (99%)	31 (1%)	62	79

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 [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](#)

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	F	601	1	14,14,15	0.73	0	17,19,21	0.58	0
6	NAG	E	601	1	14,14,15	0.45	0	17,19,21	0.80	1 (5%)
6	NAG	A	601	1	14,14,15	0.33	0	17,19,21	0.73	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	F	601	1	-	0/6/23/26	0/1/1/1
6	NAG	E	601	1	-	0/6/23/26	0/1/1/1
6	NAG	A	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	2.20	115.13	112.19
6	E	601	NAG	C1-O5-C5	2.14	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	F	601	NAG	1	0
6	A	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.

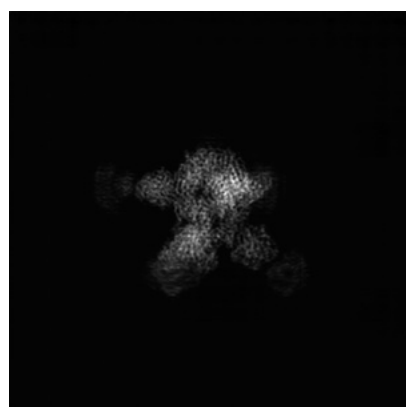
6 Map visualisation [i](#)

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.

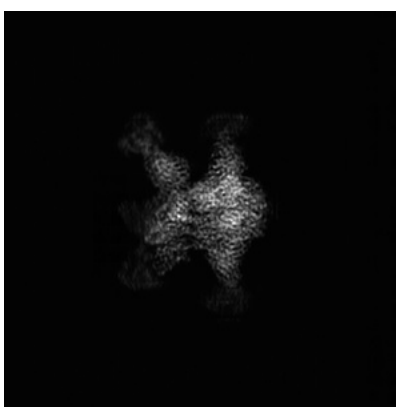
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

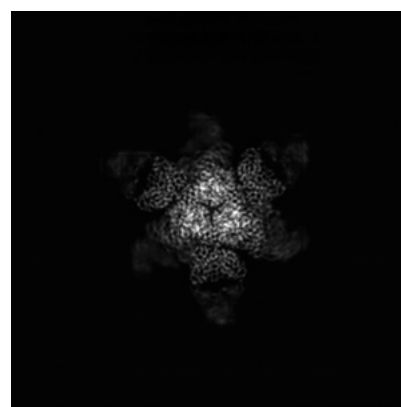
6.1.1 Primary map



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

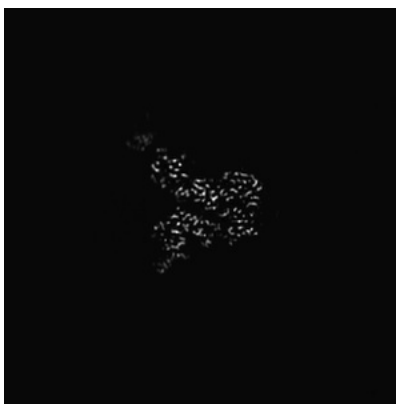
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 122



Y Index: 118

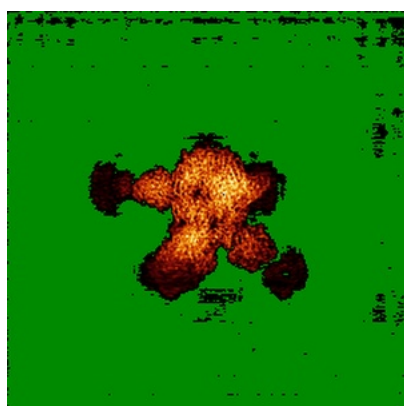


Z Index: 146

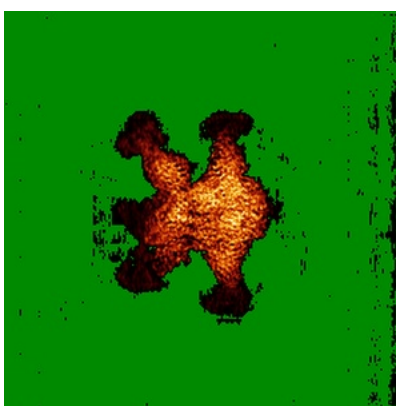
The images above show the largest variance slices of the map in three orthogonal directions.

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

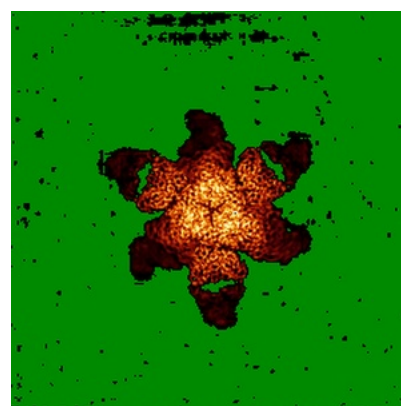
6.4.1 Primary map



X



Y

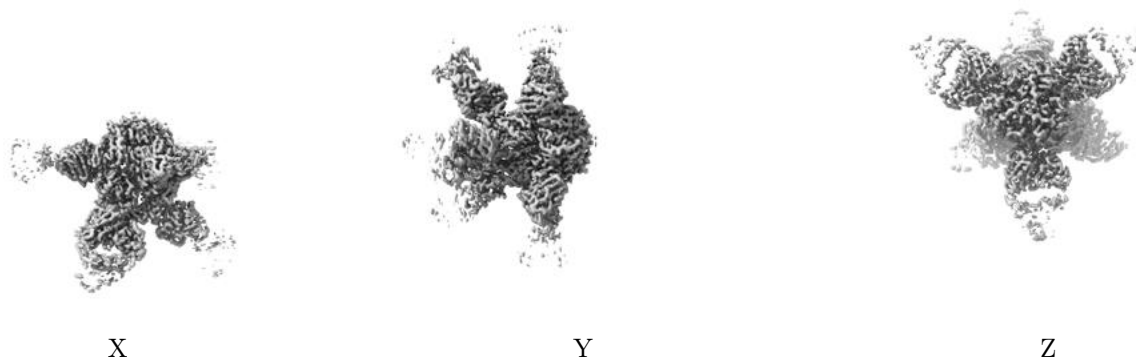


Z

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 [i](#)

6.5.1 Primary map



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.

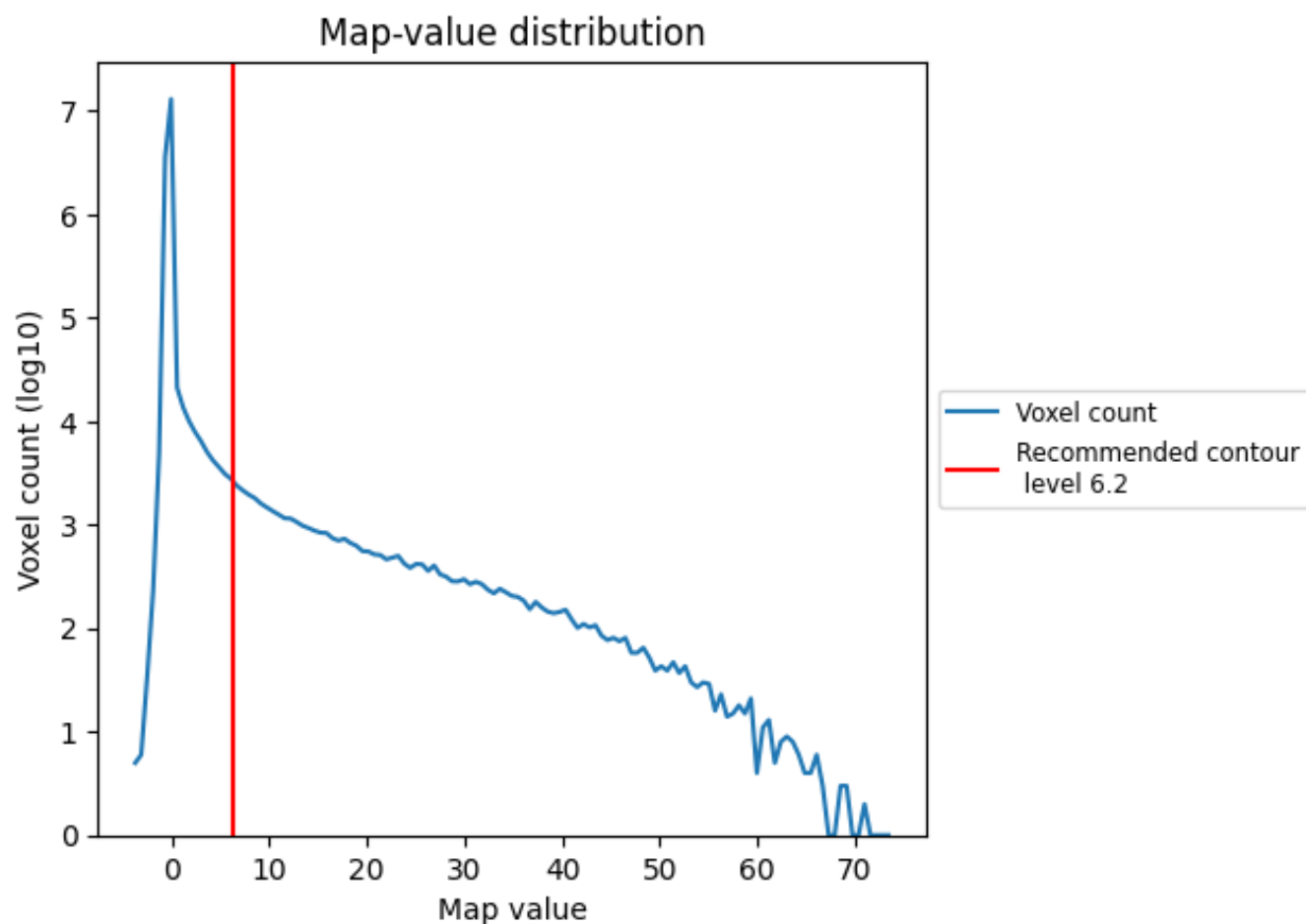
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

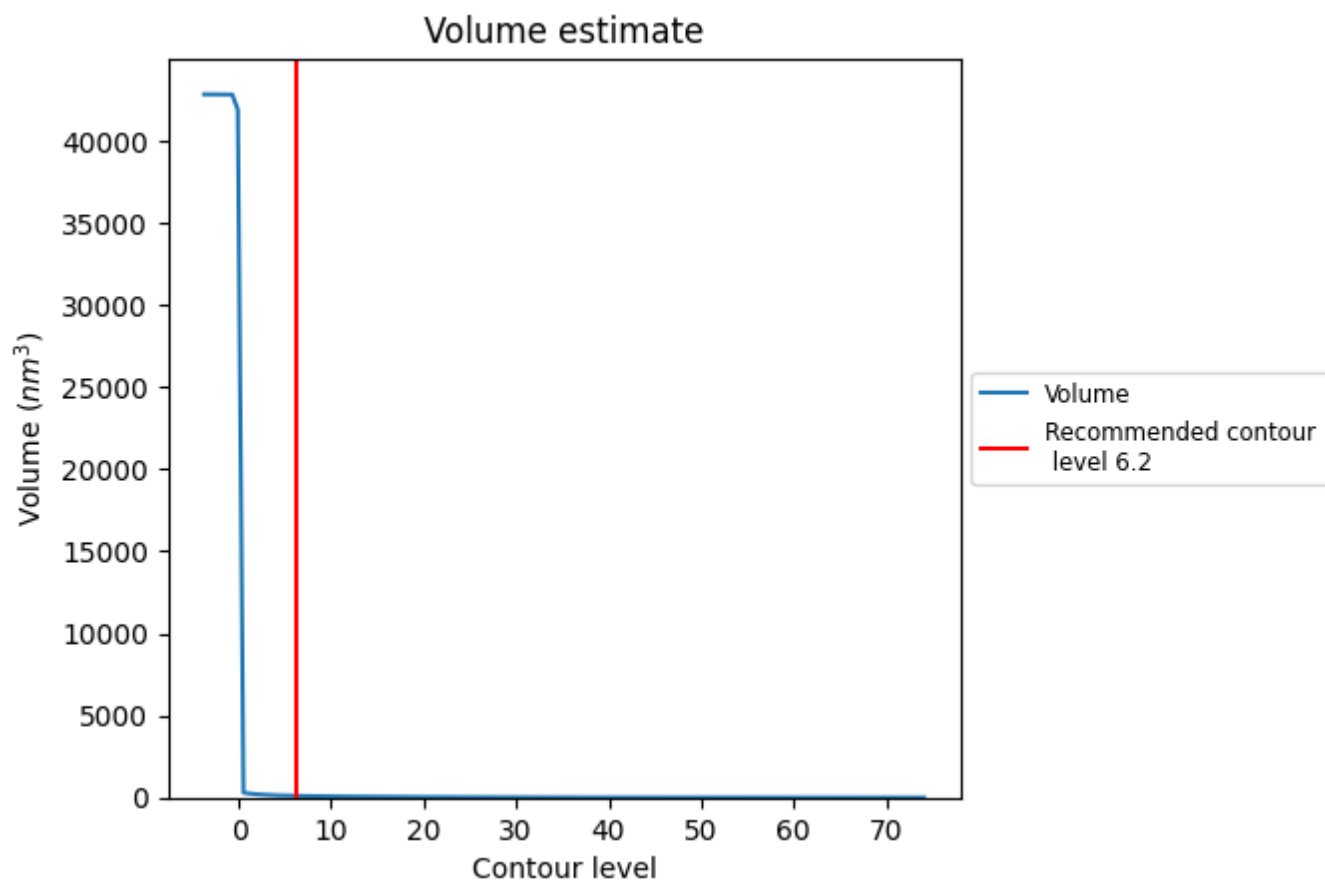
This section contains the results of statistical analysis of the map.

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.

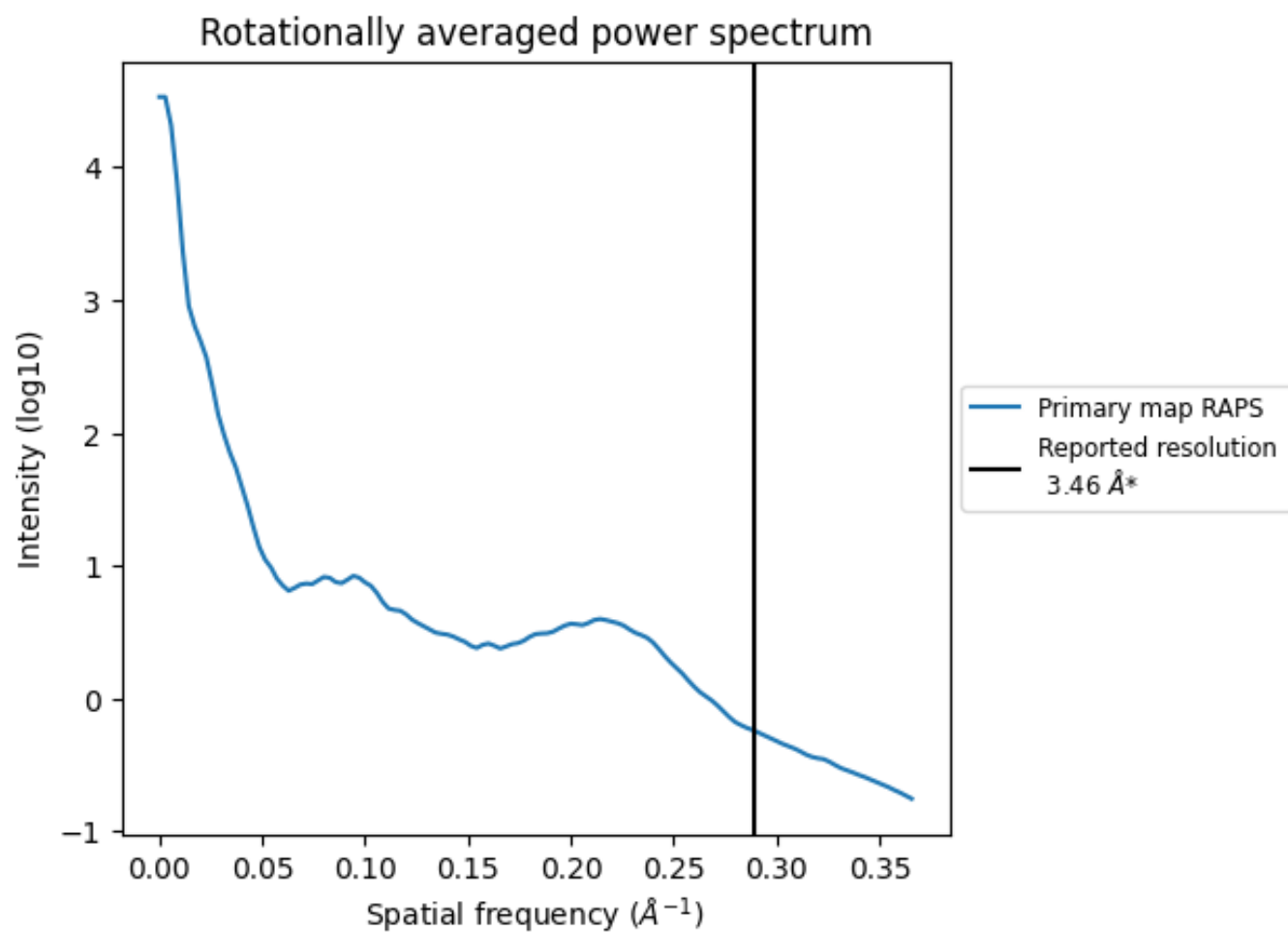
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 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⁻¹

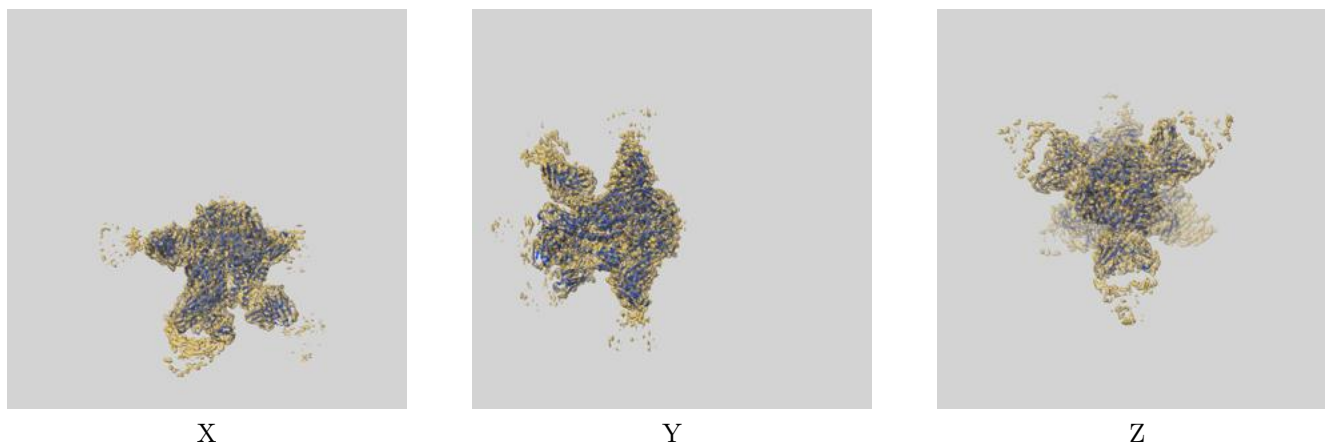
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

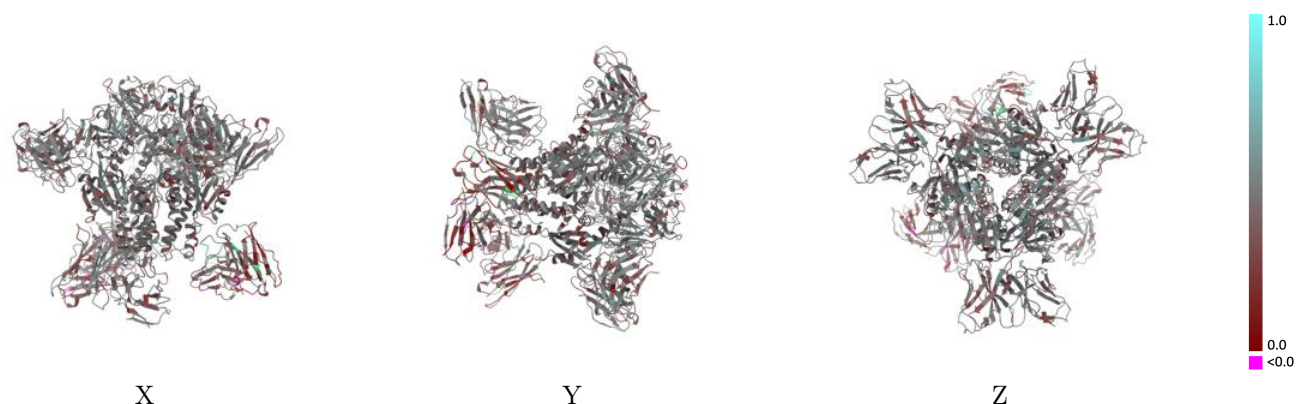
This section contains information regarding the fit between EMDB map EMD-27024 and PDB model 8CW9. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



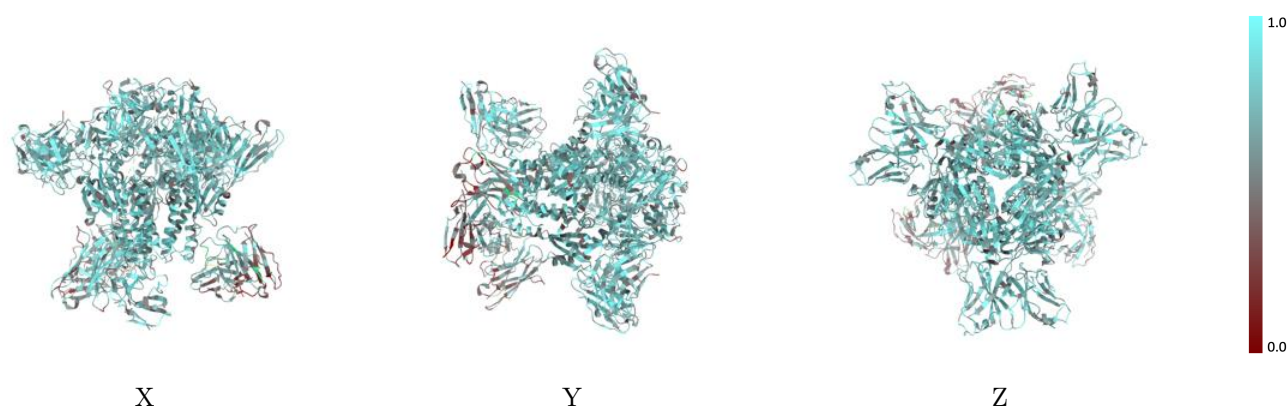
The images above show the 3D surface view of the map at the recommended contour level 6.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



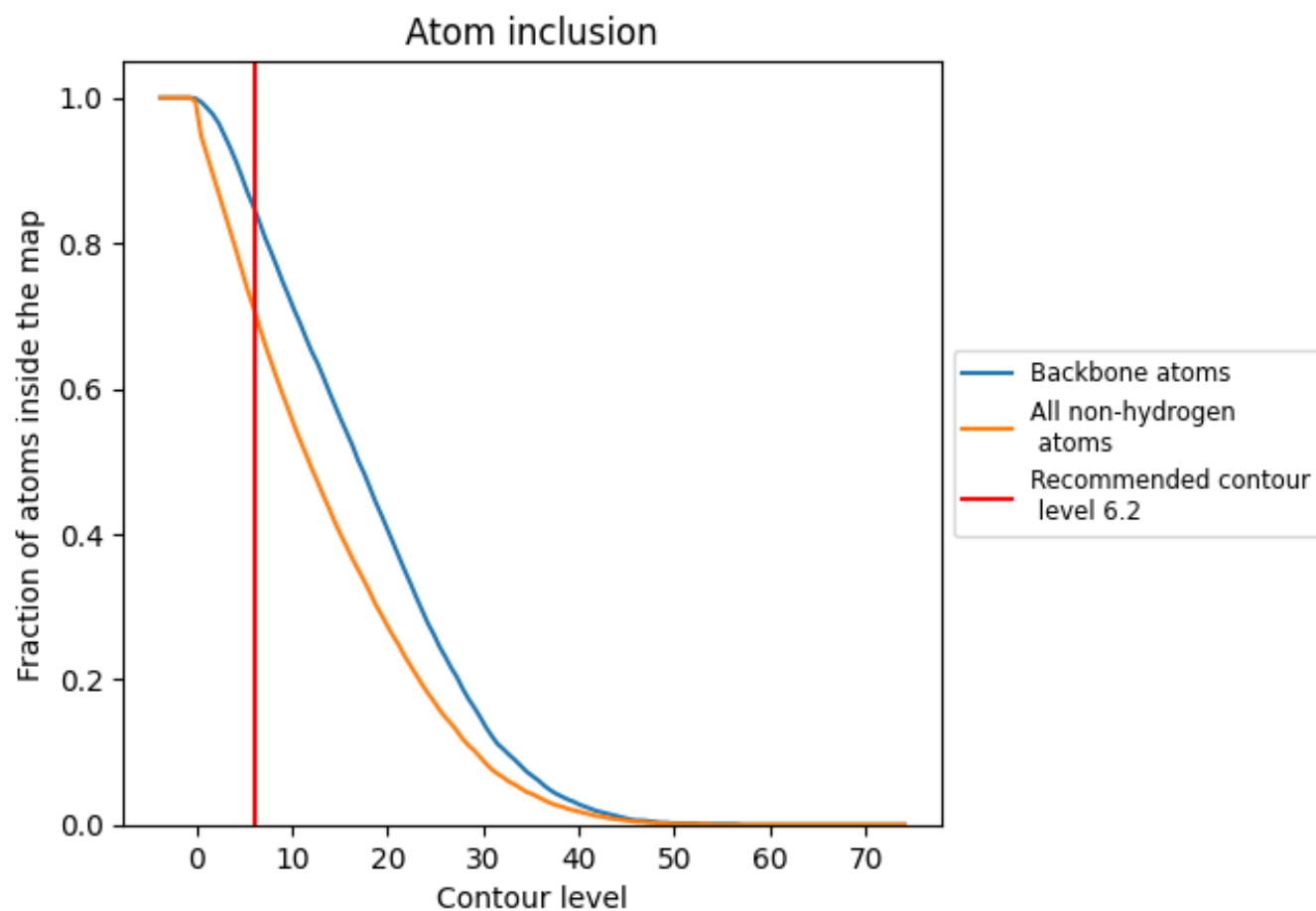
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.7030	 0.4190
A	 0.7360	 0.4490
B	 0.7240	 0.4320
C	 0.5490	 0.3140
D	 0.5480	 0.3040
E	 0.7370	 0.4470
F	 0.7490	 0.4530
G	 0.7220	 0.4280
H	 0.7150	 0.4320
I	 0.5660	 0.3250
J	 0.7420	 0.4350
K	 0.5170	 0.3090
L	 0.7050	 0.3980
M	 0.7390	 0.4400
N	 0.7510	 0.4330
O	 0.7320	 0.4320

