



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 12:21 pm GMT

PDB ID : 7NPU
EMDB ID : EMD-12521
Title : MycP5-free ESX-5 inner membrane complex, state I
Authors : Fahrenkamp, D.; Bunduc, C.M.; Wald, J.; Ummels, R.; Bitter, W.; Houben, E.N.G.; Marlovits, T.C.
Deposited on : 2021-02-28
Resolution : 4.48 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.dev43
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) : 2.31.3

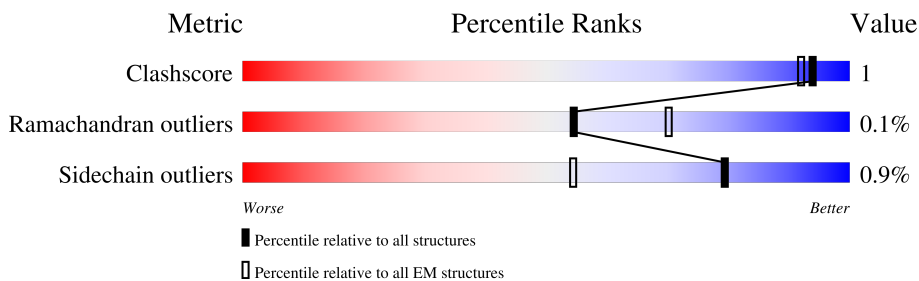
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.48 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 ≥ 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	B1	506	14% 85%
1	B2	506	14% 85%
1	B3	506	14% 85%
1	B4	506	14% 85%
1	B5	506	14% 85%
1	B6	506	14% 85%
2	C1	1391	10% 28% 71%
2	C2	1391	10% 28% 71%

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Mol	Chain	Length	Quality of chain
2	C3	1391	
2	C4	1391	
2	C5	1391	
2	C6	1391	
3	D1	503	
3	D2	503	
3	D3	503	
3	D4	503	
3	D5	503	
3	D6	503	
3	D7	503	
3	D8	503	
3	D9	503	
3	DA	503	
3	DB	503	
3	DC	503	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 126727 atoms, of which 64397 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 ESX-5 secretion system ATPase EccB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	B1	74	1147	356	585	105	98	3	0	0
1	B2	74	1147	356	585	105	98	3	0	0
1	B3	74	1147	356	585	105	98	3	0	0
1	B4	74	1147	356	585	105	98	3	0	0
1	B5	74	1147	356	585	105	98	3	0	0
1	B6	74	1147	356	585	105	98	3	0	0

- Molecule 2 is a protein called ESX-5 secretion system protein EccC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C1	406	6335	2052	3145	536	576	26	0	0
2	C2	406	6335	2052	3145	536	576	26	0	0
2	C3	406	6335	2052	3145	536	576	26	0	0
2	C4	406	6335	2052	3145	536	576	26	0	0
2	C5	406	6335	2052	3145	536	576	26	0	0
2	C6	406	6335	2052	3145	536	576	26	0	0

- Molecule 3 is a protein called ESX-5 secretion system protein EccD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D1	485	7458	2353	3823	633	628	21	0	0

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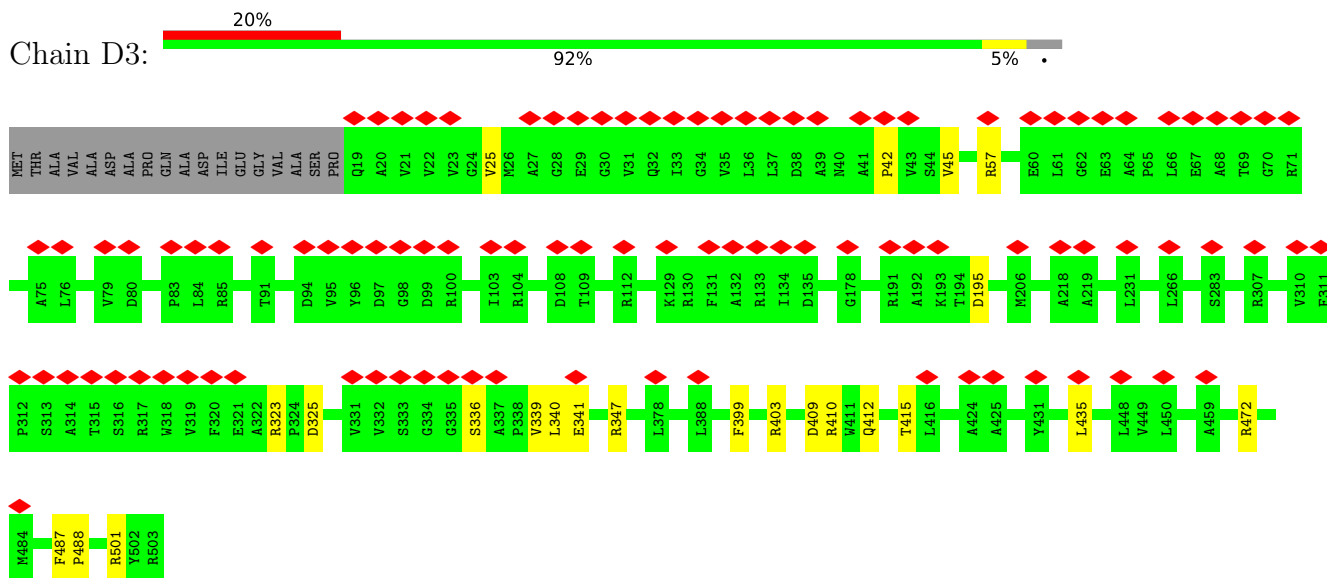
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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	D2	405	Total 6155	C 1919	H 3166	N 528	O 524	S 18	0	0
3	D3	485	Total 7459	C 2353	H 3824	N 633	O 628	S 21	0	0
3	D4	415	Total 6308	C 1969	H 3245	N 541	O 535	S 18	0	0
3	D5	485	Total 7459	C 2353	H 3824	N 633	O 628	S 21	0	0
3	D6	405	Total 6155	C 1919	H 3166	N 528	O 524	S 18	0	0
3	D7	485	Total 7459	C 2353	H 3824	N 633	O 628	S 21	0	0
3	D8	405	Total 6154	C 1919	H 3165	N 528	O 524	S 18	0	0
3	D9	485	Total 7459	C 2353	H 3824	N 633	O 628	S 21	0	0
3	DA	405	Total 6156	C 1919	H 3167	N 528	O 524	S 18	0	0
3	DB	485	Total 7459	C 2353	H 3824	N 633	O 628	S 21	0	0
3	DC	405	Total 6154	C 1919	H 3165	N 528	O 524	S 18	0	0

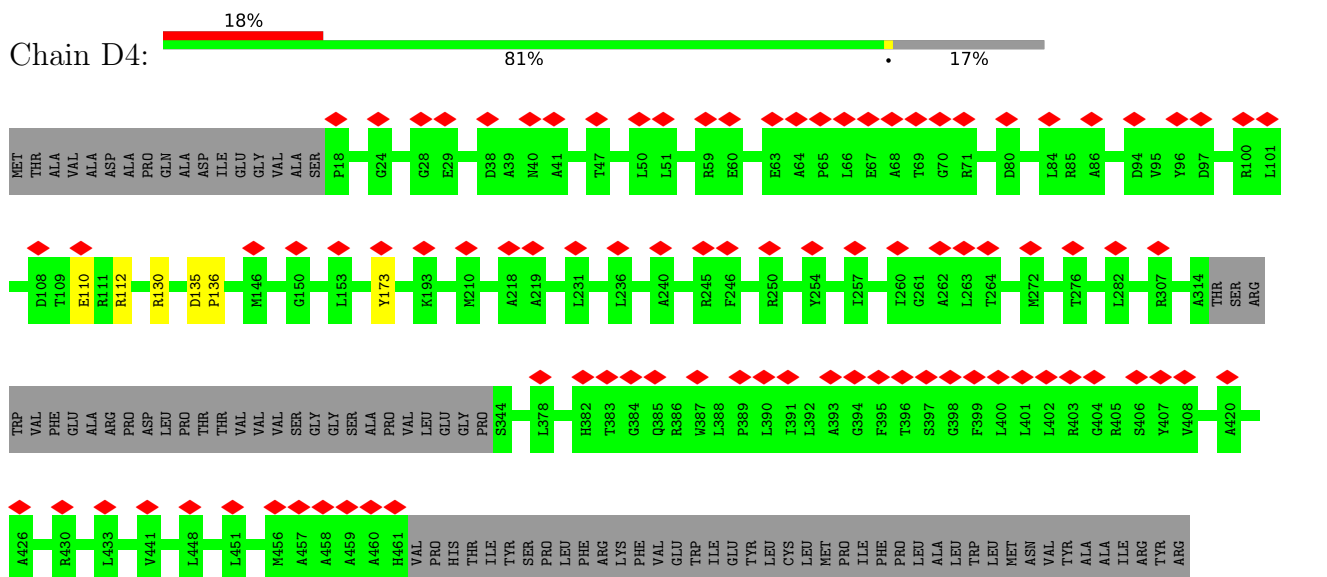
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VAL	ALA	HIS	ILE	GLY	ARG	ASP	ILE	LEU	VAL	MET	SER	PRO	GLY	ASN	ILE	LEU	PHE	VAL	ALA	TRP	LEU	THR	THR	ASP	THR	THR	GLY	ARG	LEU	GLN	ARG	ALA	PRO	PHE	GLY	ASN	ASP	LEU	VAL	LEU	PHE	PRO	PHE	LEU	ASP	GLY	GLU	VAL	LEU	PRO	HIS	
ASP	GLU	GLY	ILE	ASP	PRO	HIS	LEU	SER	GLU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

● Molecule 2: ESX-5 secretion system protein EccC5

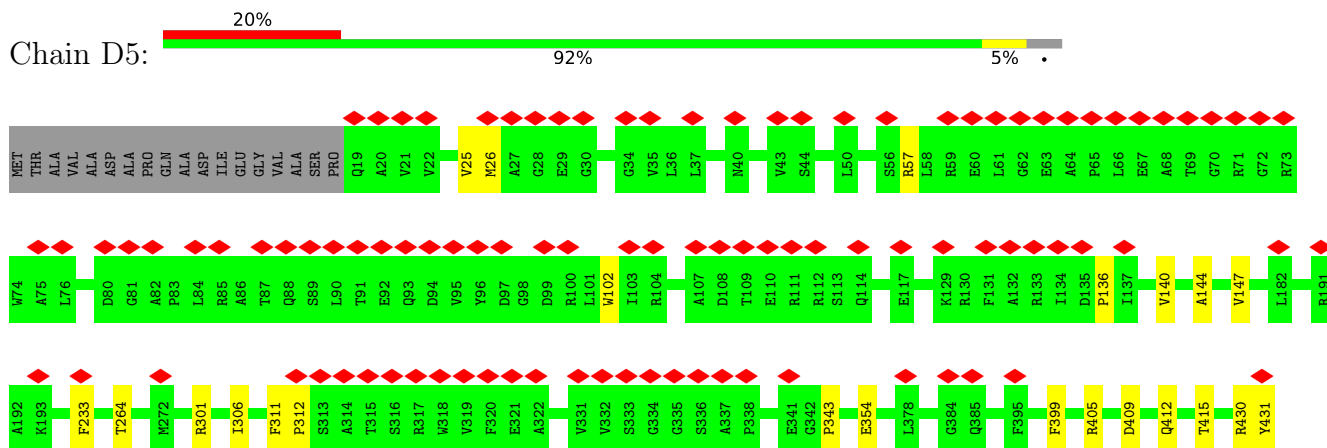


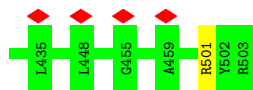


• Molecule 3: ESX-5 secretion system protein EccD5

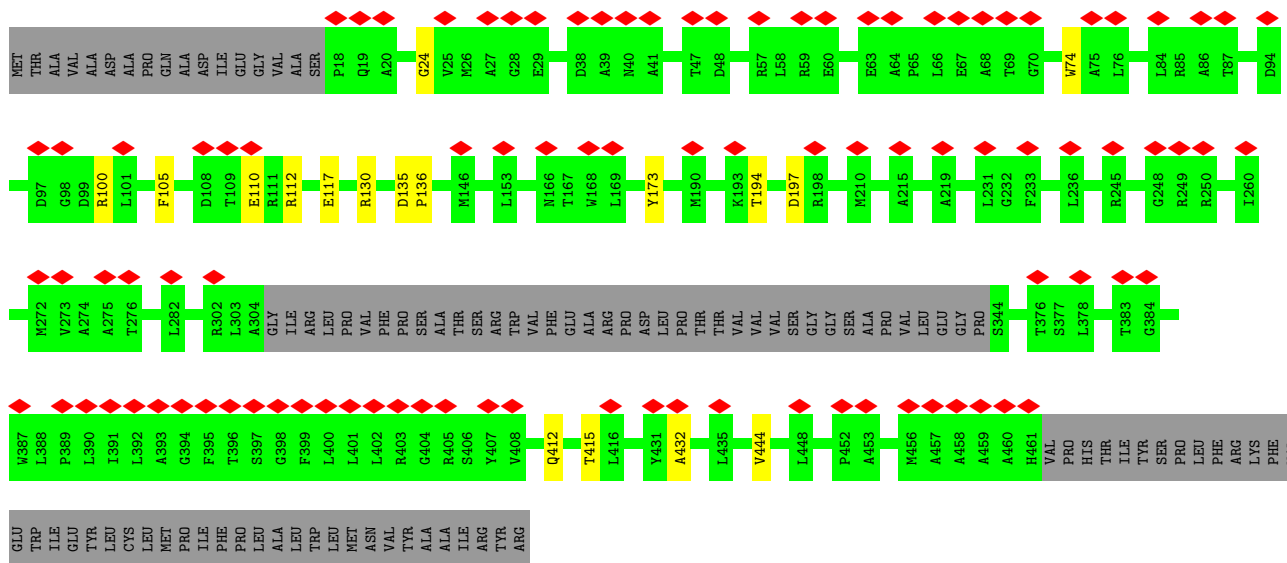
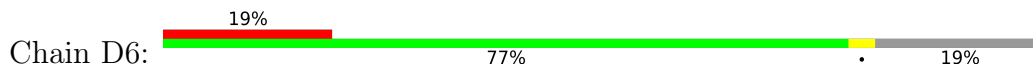


• Molecule 3: ESX-5 secretion system protein EccD5

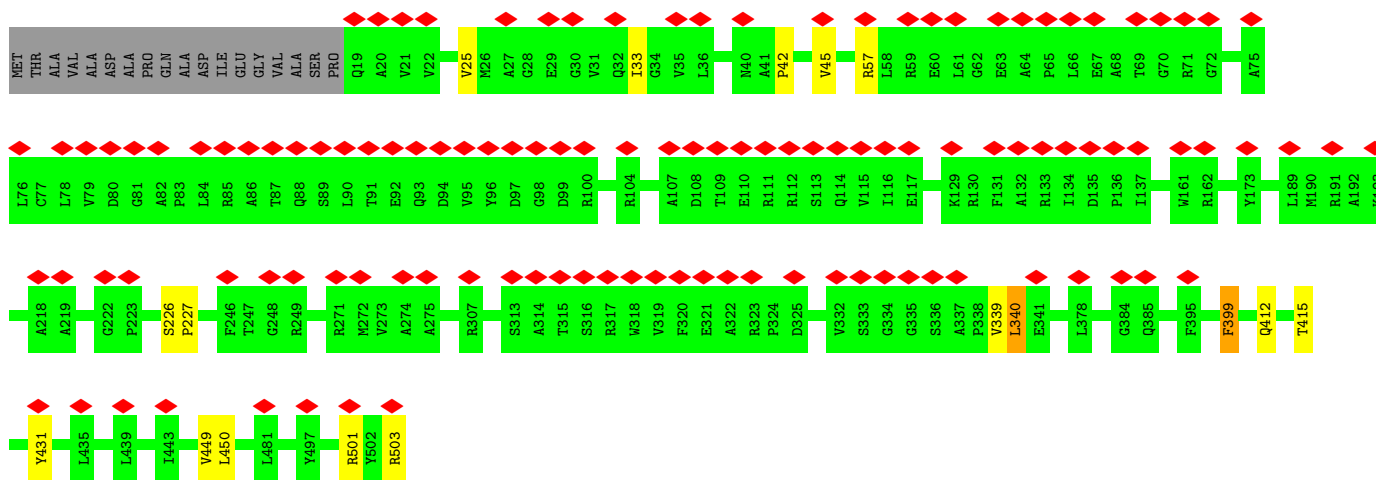




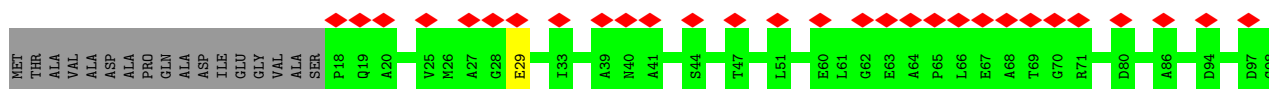
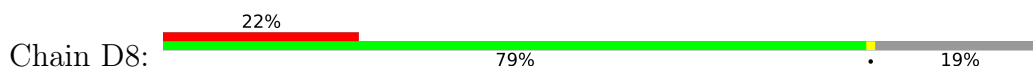
• Molecule 3: ESX-5 secretion system protein EccD5

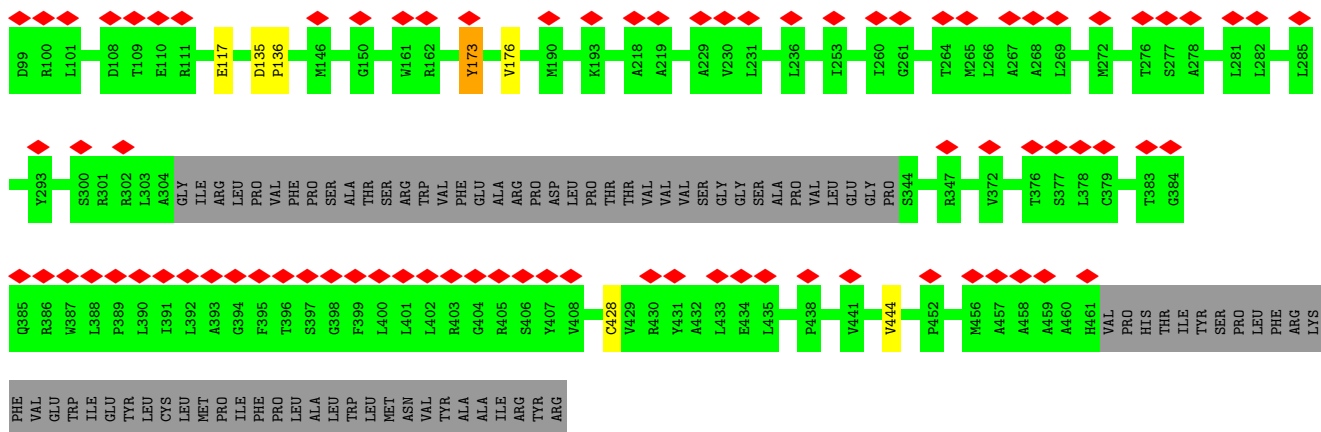


• Molecule 3: ESX-5 secretion system protein EccD5

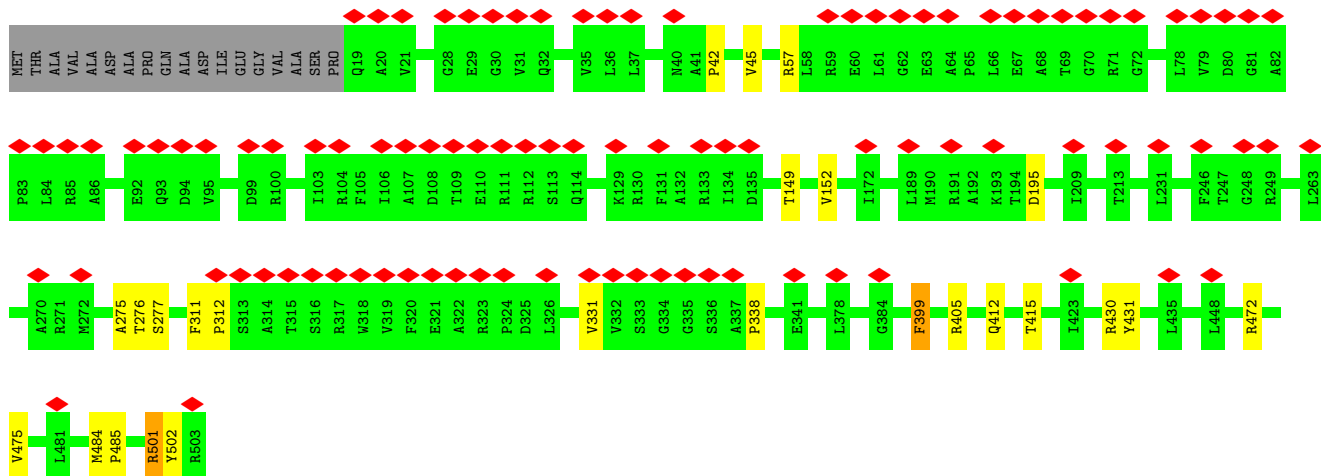


• Molecule 3: ESX-5 secretion system protein EccD5

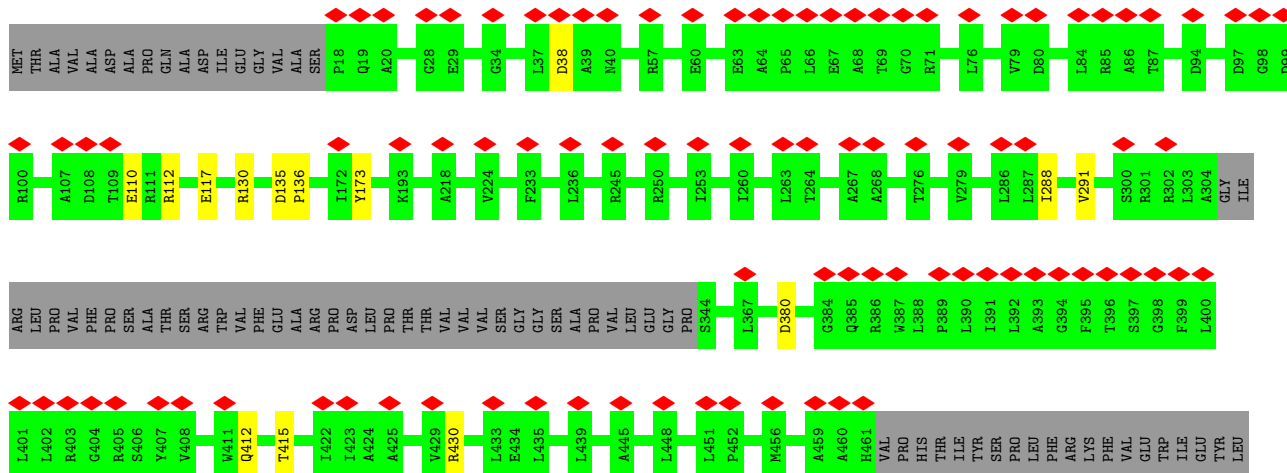
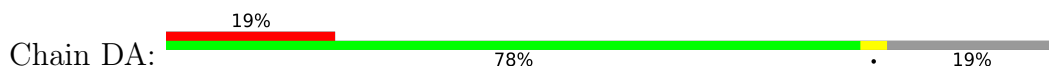




● Molecule 3: ESX-5 secretion system protein EccD5

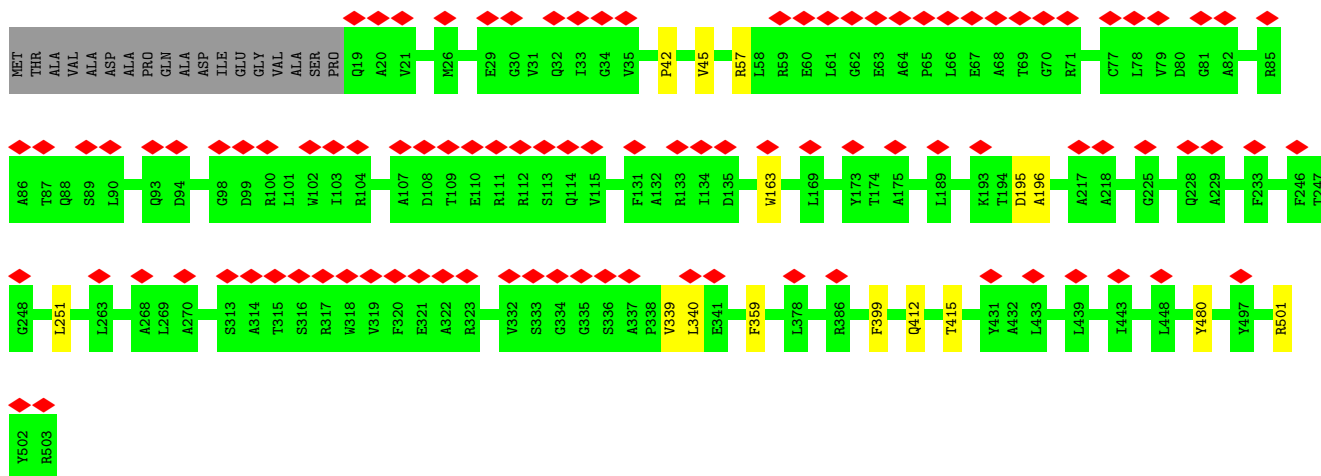


● Molecule 3: ESX-5 secretion system protein EccD5

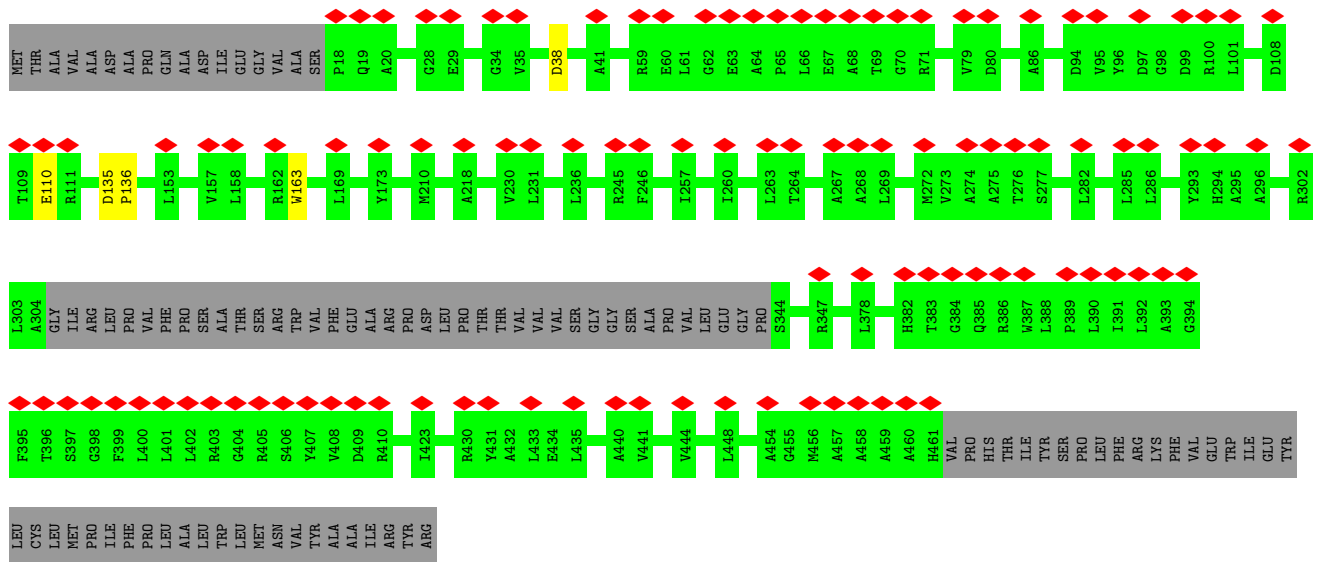
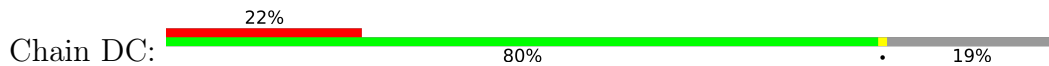


CYS
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• Molecule 3: ESX-5 secretion system protein EccD5



• Molecule 3: ESX-5 secretion system protein EccD5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	226793	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B1	0.53	0/571	0.68	0/773
1	B2	0.50	0/571	0.67	0/773
1	B3	0.50	0/571	0.72	0/773
1	B4	0.53	0/571	0.69	0/773
1	B5	0.56	0/571	0.71	0/773
1	B6	0.54	0/571	0.75	0/773
2	C1	0.38	0/3280	0.66	0/4459
2	C2	0.39	0/3280	0.64	0/4459
2	C3	0.40	0/3280	0.67	1/4459 (0.0%)
2	C4	0.39	0/3280	0.65	0/4459
2	C5	0.39	0/3280	0.64	0/4459
2	C6	0.40	0/3280	0.66	0/4459
3	D1	0.43	0/3710	0.64	0/5078
3	D2	0.36	0/3038	0.62	0/4151
3	D3	0.43	0/3710	0.65	0/5078
3	D4	0.36	0/3115	0.63	0/4257
3	D5	0.45	0/3710	0.64	0/5078
3	D6	0.35	0/3038	0.61	0/4151
3	D7	0.42	0/3710	0.63	0/5078
3	D8	0.35	0/3038	0.62	0/4151
3	D9	0.44	0/3710	0.63	0/5078
3	DA	0.36	0/3038	0.61	0/4151
3	DB	0.42	0/3710	0.65	0/5078
3	DC	0.36	0/3038	0.61	0/4151
All	All	0.40	0/63671	0.64	1/86872 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C3	37	TRP	CA-CB-CG	5.06	123.32	113.70

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	B1	562	585	584	2	0
1	B2	562	585	584	2	0
1	B3	562	585	584	2	0
1	B4	562	585	584	0	0
1	B5	562	585	584	3	0
1	B6	562	585	584	2	0
2	C1	3190	3145	3142	8	0
2	C2	3190	3145	3142	9	0
2	C3	3190	3145	3142	10	0
2	C4	3190	3145	3142	13	0
2	C5	3190	3145	3142	13	0
2	C6	3190	3145	3142	12	0
3	D1	3635	3823	3822	12	0
3	D2	2989	3166	3163	7	0
3	D3	3635	3824	3822	14	0
3	D4	3063	3245	3243	3	0
3	D5	3635	3824	3822	12	0
3	D6	2989	3166	3163	9	0
3	D7	3635	3824	3822	8	0
3	D8	2989	3165	3163	3	0
3	D9	3635	3824	3822	13	0
3	DA	2989	3167	3163	7	0
3	DB	3635	3824	3822	7	0
3	DC	2989	3165	3163	3	0
All	All	62330	64397	64346	157	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 1.

The worst 5 of 157 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C3:130:ARG:NH2	3:DC:110:GLU:OE2	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C4:130:ARG:NH2	3:DA:110:GLU:OE2	2.20	0.73
3:D1:354:GLU:OE1	3:D2:130:ARG:NH1	2.22	0.70
3:D9:412:GLN:O	3:D9:415:THR:HG22	1.95	0.67
2:C5:185:ASP:OD1	2:C5:186:ILE:N	2.31	0.63

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	B1	72/506 (14%)	68 (94%)	4 (6%)	0	100	100
1	B2	72/506 (14%)	71 (99%)	1 (1%)	0	100	100
1	B3	72/506 (14%)	68 (94%)	4 (6%)	0	100	100
1	B4	72/506 (14%)	72 (100%)	0	0	100	100
1	B5	72/506 (14%)	72 (100%)	0	0	100	100
1	B6	72/506 (14%)	71 (99%)	1 (1%)	0	100	100
2	C1	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	47	81
2	C2	402/1391 (29%)	394 (98%)	7 (2%)	1 (0%)	47	81
2	C3	402/1391 (29%)	389 (97%)	12 (3%)	1 (0%)	47	81
2	C4	402/1391 (29%)	390 (97%)	11 (3%)	1 (0%)	47	81
2	C5	402/1391 (29%)	394 (98%)	6 (2%)	2 (0%)	29	68
2	C6	402/1391 (29%)	391 (97%)	10 (2%)	1 (0%)	47	81
3	D1	483/503 (96%)	477 (99%)	6 (1%)	0	100	100
3	D2	401/503 (80%)	396 (99%)	5 (1%)	0	100	100
3	D3	483/503 (96%)	474 (98%)	8 (2%)	1 (0%)	47	81
3	D4	411/503 (82%)	404 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D5	483/503 (96%)	472 (98%)	11 (2%)	0	100	100
3	D6	401/503 (80%)	396 (99%)	5 (1%)	0	100	100
3	D7	483/503 (96%)	474 (98%)	9 (2%)	0	100	100
3	D8	401/503 (80%)	394 (98%)	6 (2%)	1 (0%)	47	81
3	D9	483/503 (96%)	475 (98%)	8 (2%)	0	100	100
3	DA	401/503 (80%)	394 (98%)	7 (2%)	0	100	100
3	DB	483/503 (96%)	476 (99%)	7 (1%)	0	100	100
3	DC	401/503 (80%)	396 (99%)	5 (1%)	0	100	100
All	All	8158/17418 (47%)	8000 (98%)	149 (2%)	9 (0%)	54	85

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C1	155	GLY
2	C5	154	ASP
2	C4	155	GLY
3	D3	336	SER
3	D8	29	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	58/411 (14%)	58 (100%)	0	100	100
1	B2	58/411 (14%)	58 (100%)	0	100	100
1	B3	58/411 (14%)	58 (100%)	0	100	100
1	B4	58/411 (14%)	57 (98%)	1 (2%)	60	78
1	B5	58/411 (14%)	58 (100%)	0	100	100
1	B6	58/411 (14%)	58 (100%)	0	100	100
2	C1	342/1137 (30%)	340 (99%)	2 (1%)	86	92
2	C2	342/1137 (30%)	339 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C3	342/1137 (30%)	340 (99%)	2 (1%)	86	92
2	C4	342/1137 (30%)	338 (99%)	4 (1%)	71	84
2	C5	342/1137 (30%)	337 (98%)	5 (2%)	65	80
2	C6	342/1137 (30%)	339 (99%)	3 (1%)	78	87
3	D1	381/393 (97%)	376 (99%)	5 (1%)	69	82
3	D2	311/393 (79%)	309 (99%)	2 (1%)	86	92
3	D3	381/393 (97%)	377 (99%)	4 (1%)	76	86
3	D4	319/393 (81%)	317 (99%)	2 (1%)	86	92
3	D5	381/393 (97%)	376 (99%)	5 (1%)	69	82
3	D6	311/393 (79%)	309 (99%)	2 (1%)	86	92
3	D7	381/393 (97%)	376 (99%)	5 (1%)	69	82
3	D8	311/393 (79%)	309 (99%)	2 (1%)	86	92
3	D9	381/393 (97%)	376 (99%)	5 (1%)	69	82
3	DA	311/393 (79%)	308 (99%)	3 (1%)	76	86
3	DB	381/393 (97%)	377 (99%)	4 (1%)	76	86
3	DC	311/393 (79%)	310 (100%)	1 (0%)	92	95
All	All	6560/14004 (47%)	6500 (99%)	60 (1%)	79	87

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D3	399	PHE
3	DB	57	ARG
3	D5	405	ARG
3	DA	173	TYR
3	DC	163	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	D7	461	HIS
3	D7	464	HIS
3	D9	464	HIS
3	D9	165	HIS
3	D4	118	HIS

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 monosaccharides 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.

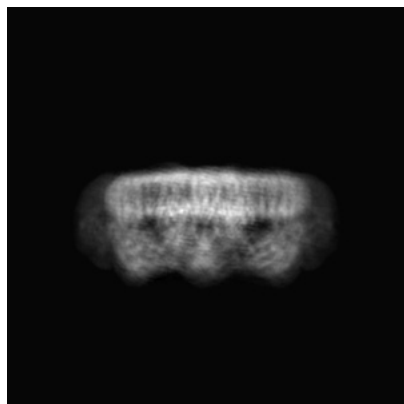
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12521. These allow visual inspection of the internal detail of the map and identification of artifacts.

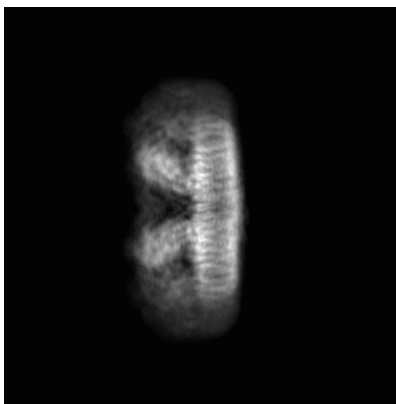
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

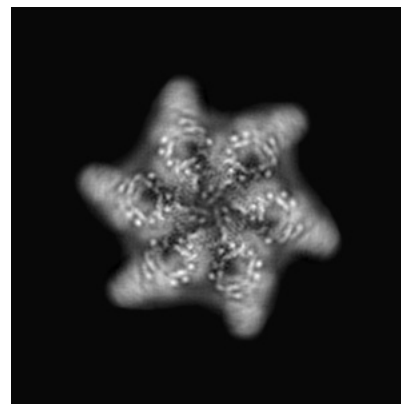
6.1.1 Primary map



X

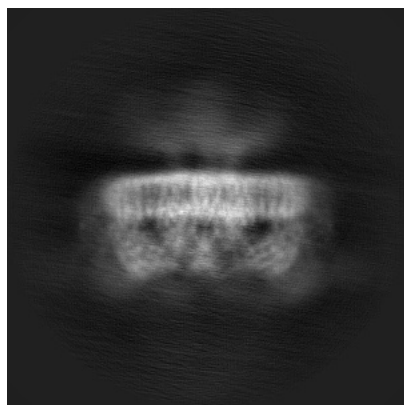


Y

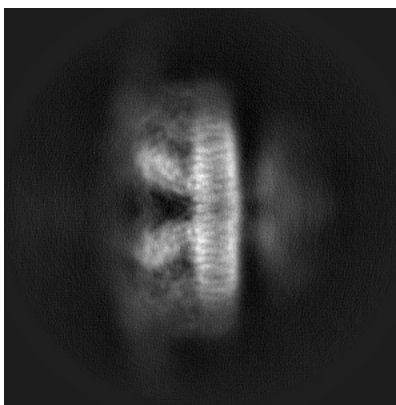


Z

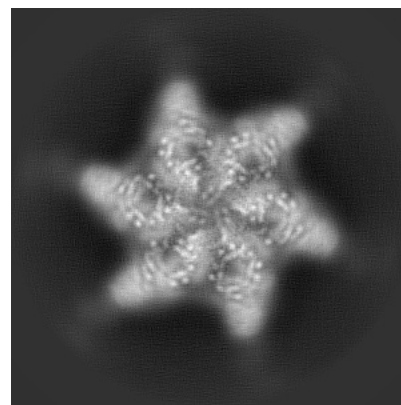
6.1.2 Raw map



X



Y



Z

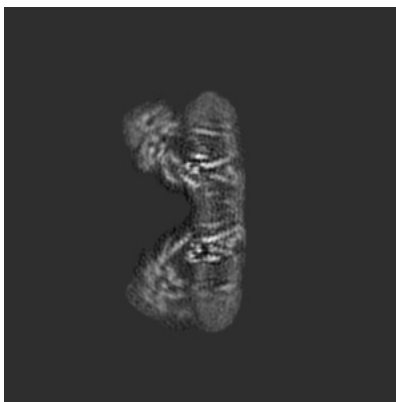
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

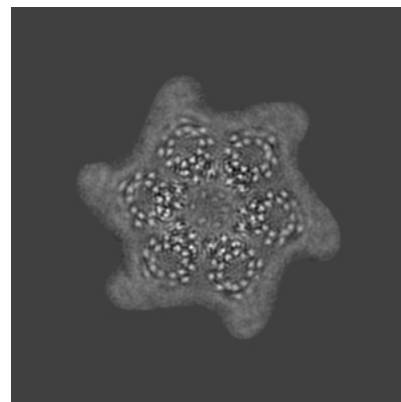
6.2.1 Primary map



X Index: 200

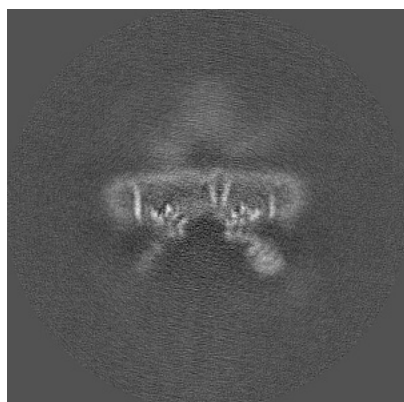


Y Index: 200

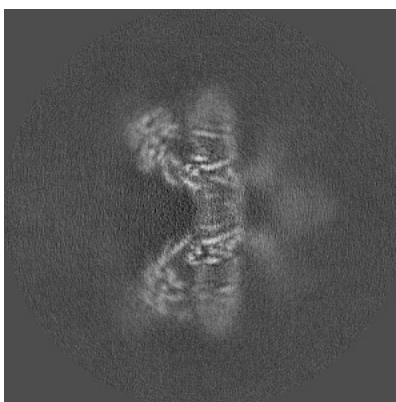


Z Index: 200

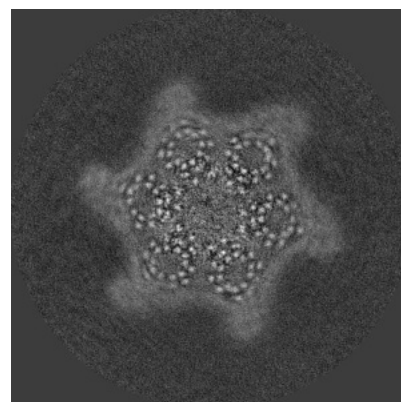
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

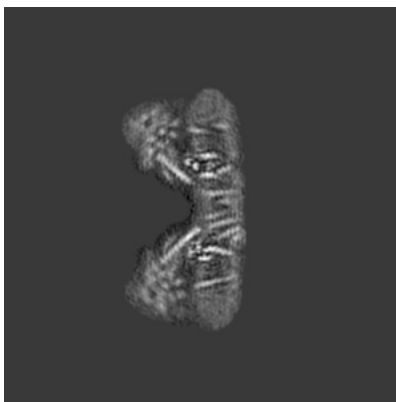
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

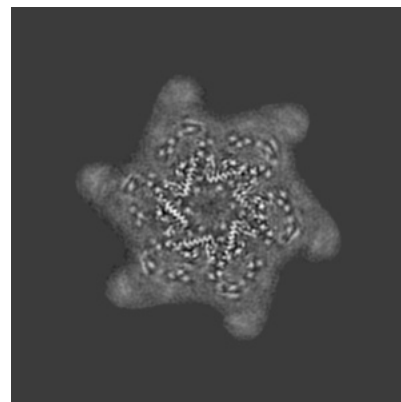
6.3.1 Primary map



X Index: 231

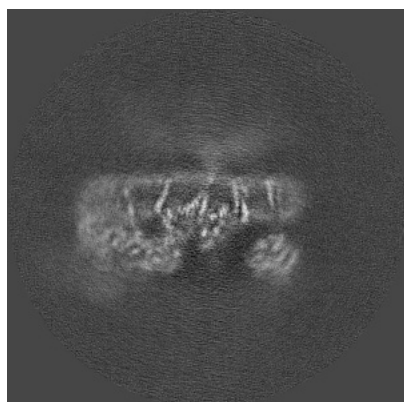


Y Index: 197

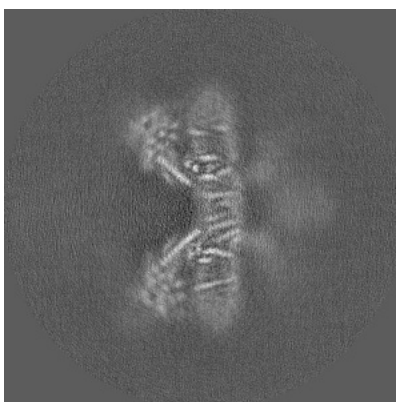


Z Index: 194

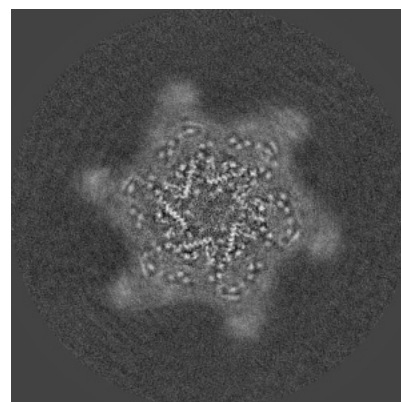
6.3.2 Raw map



X Index: 232



Y Index: 197



Z Index: 194

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



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

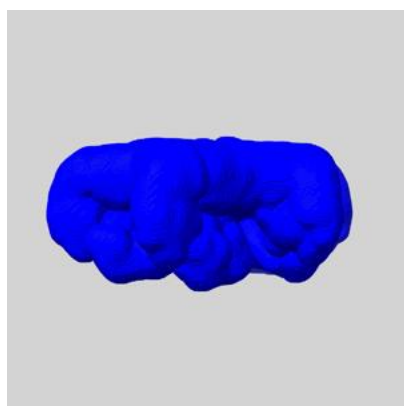
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

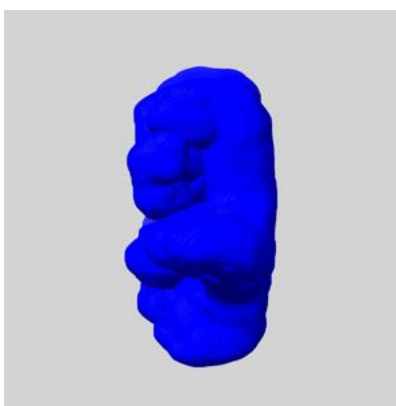
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

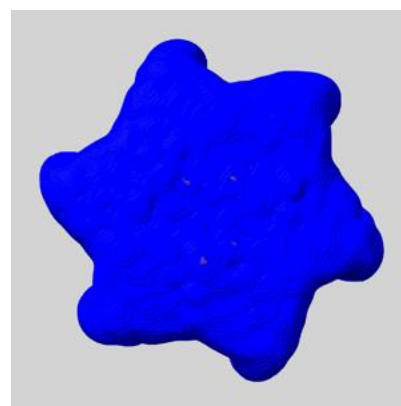
6.5.1 emd_12521_msk_1.map [i](#)



X



Y

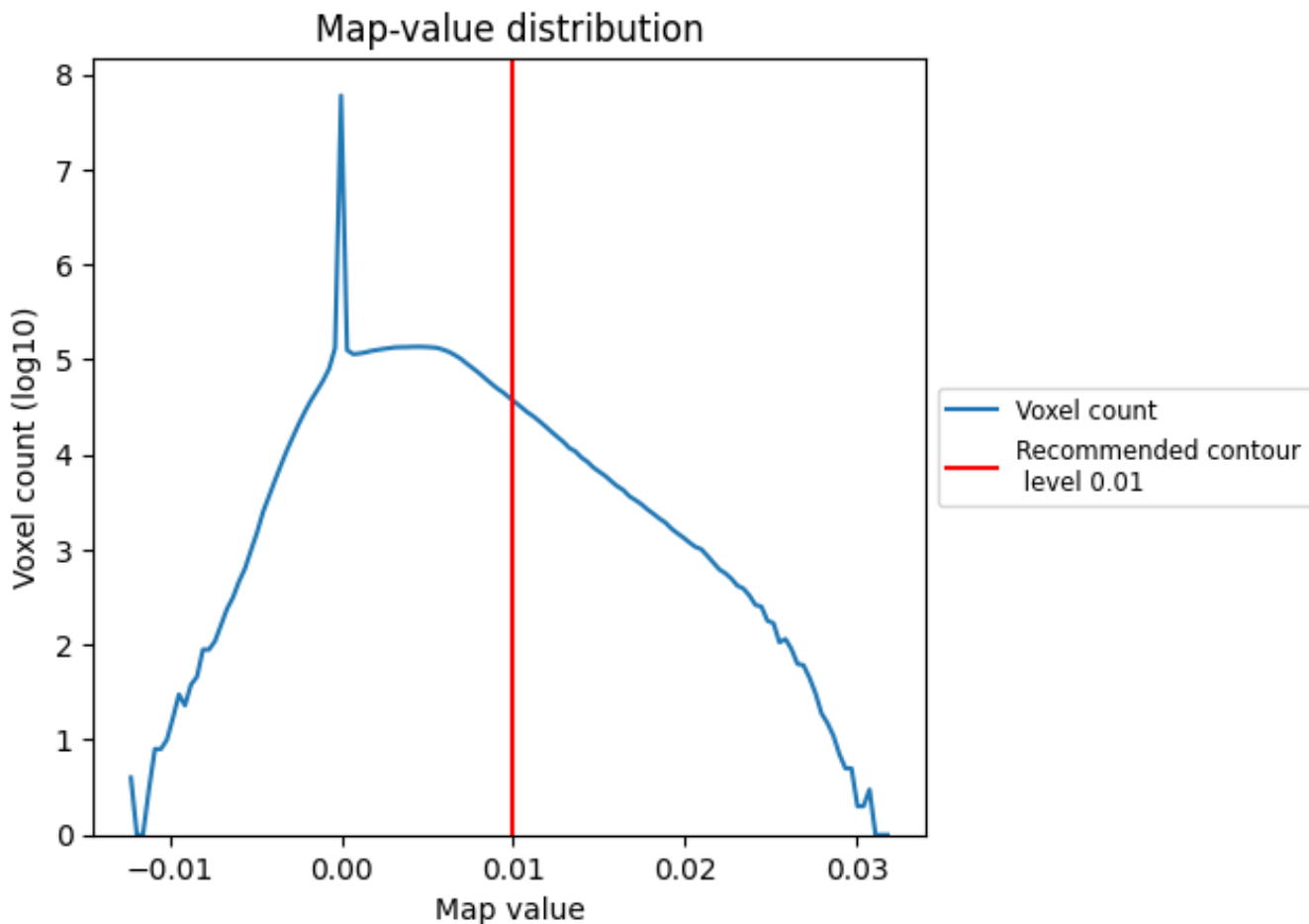


Z

7 Map analysis [i](#)

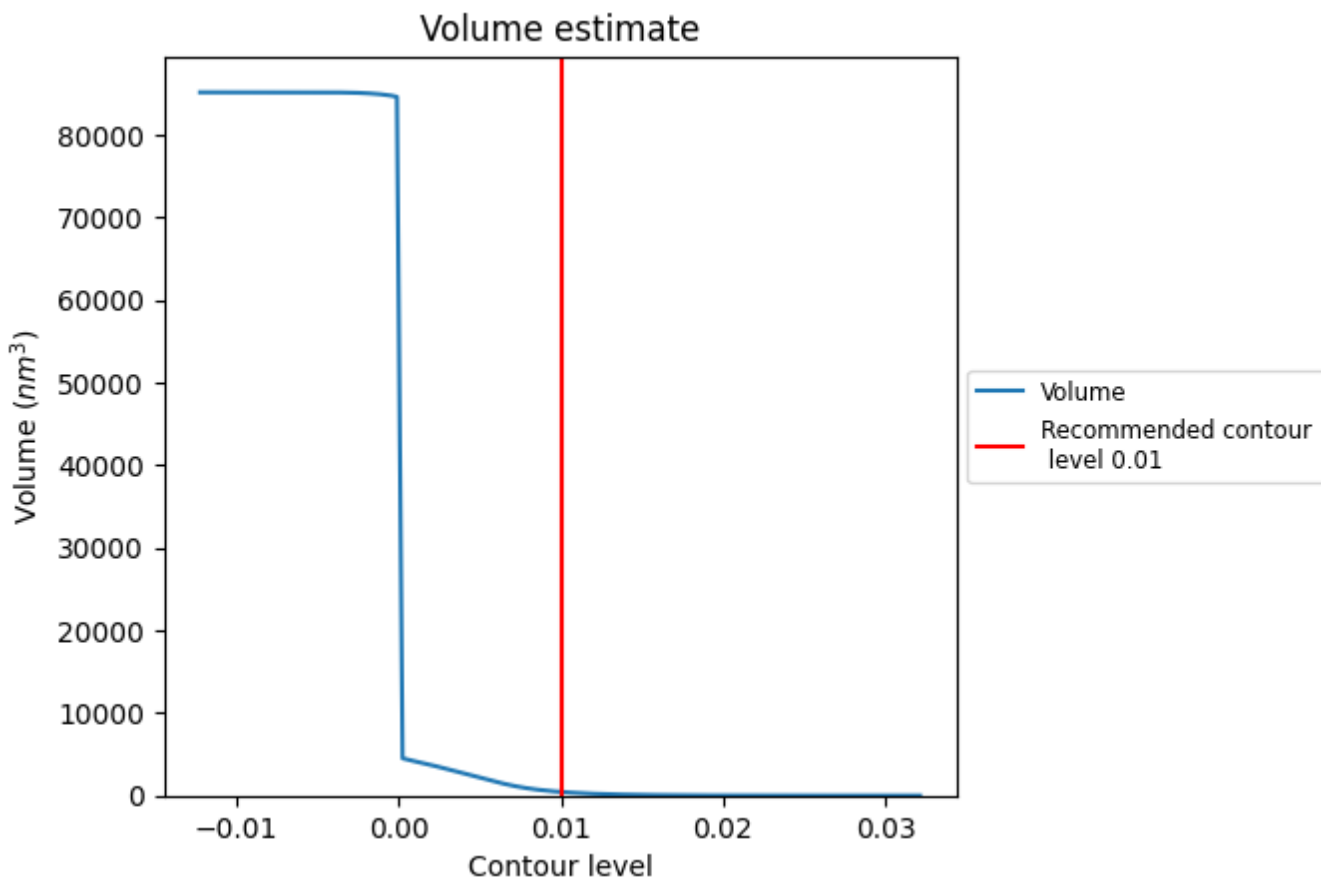
This section contains the results of statistical analysis of the map.

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.

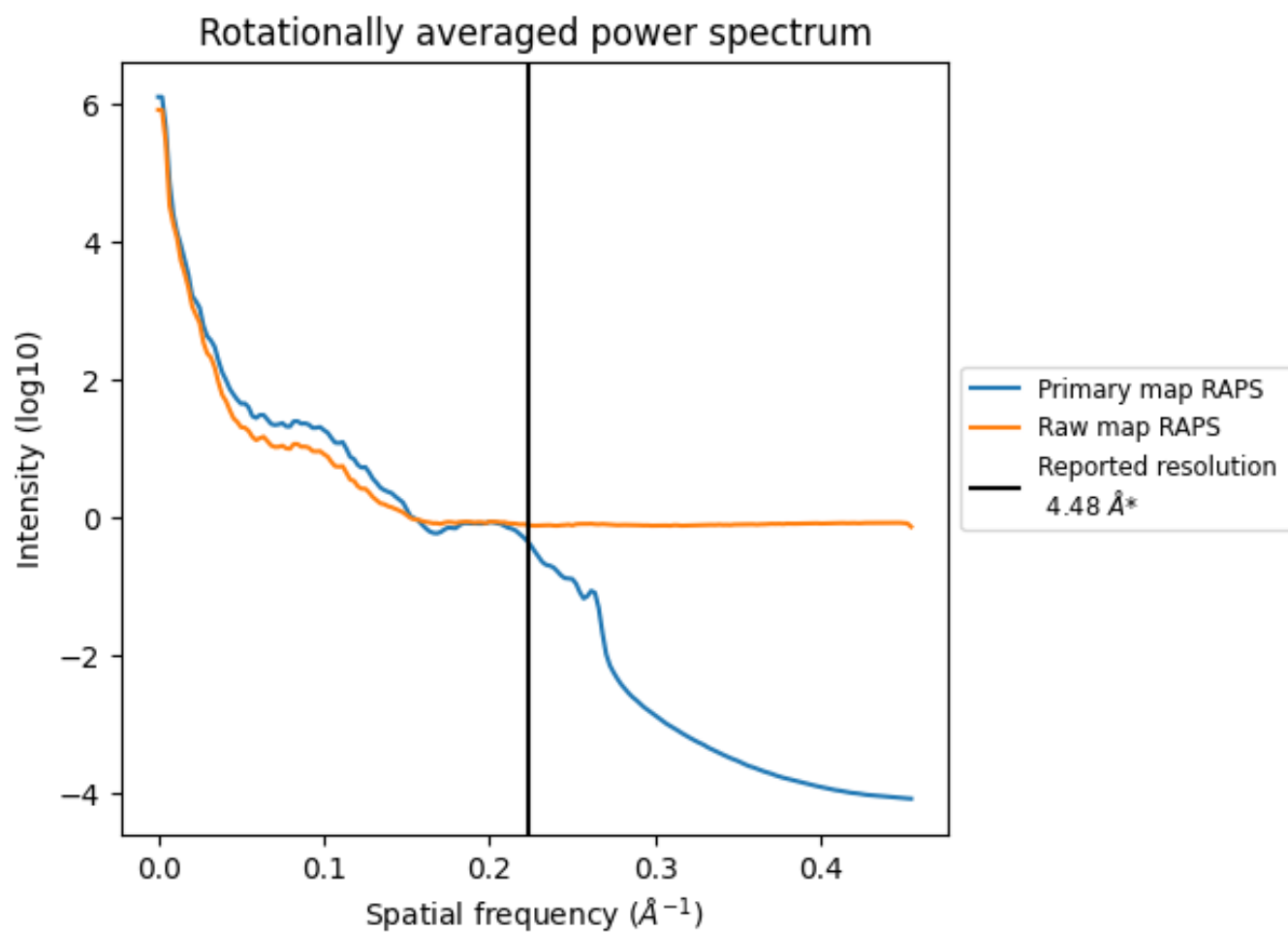
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 440 nm³; this corresponds to an approximate mass of 397 kDa.

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

7.3 Rotationally averaged power spectrum i

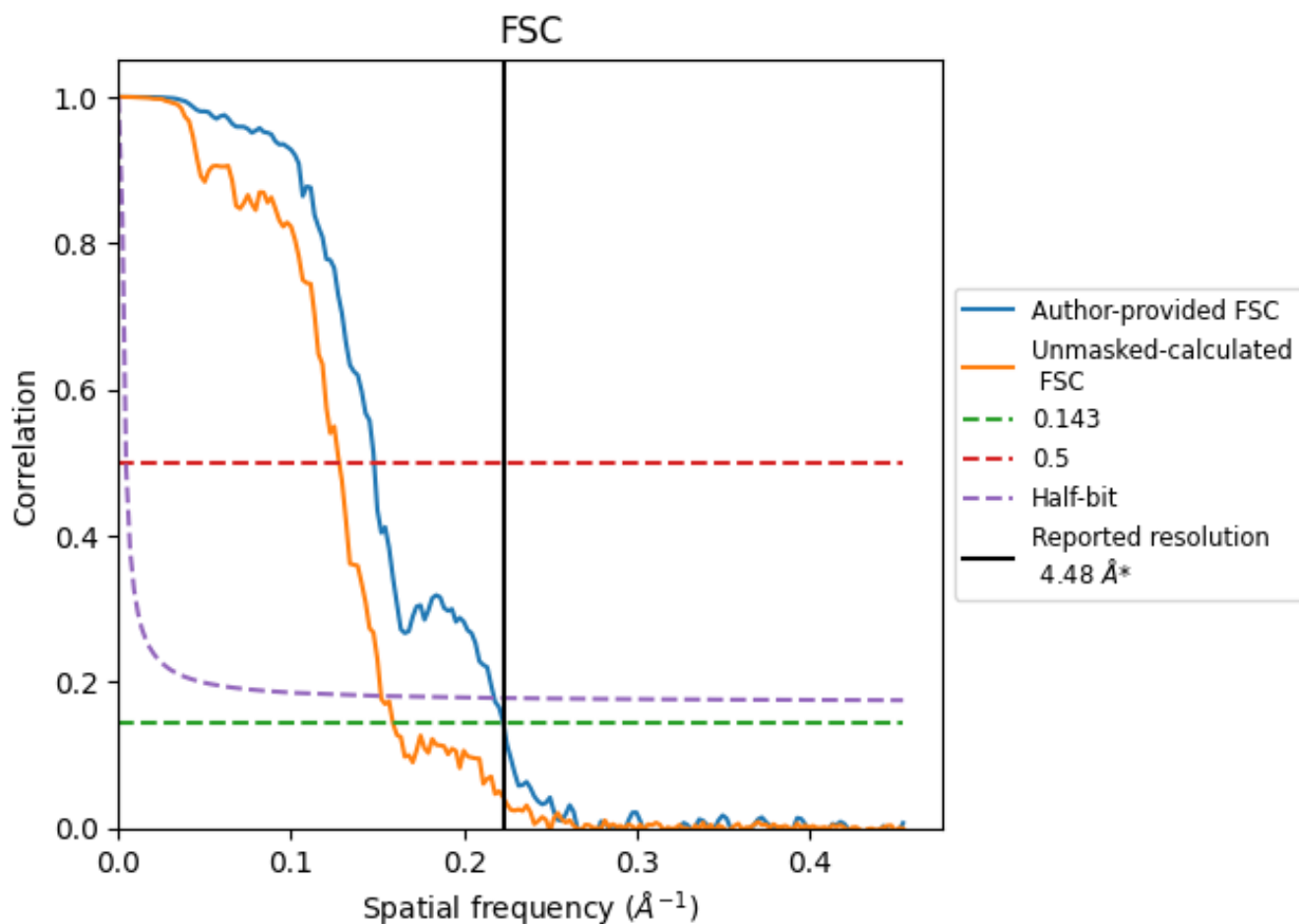


*Reported resolution corresponds to spatial frequency of 0.223 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.223 Å⁻¹

8.2 Resolution estimates [i](#)

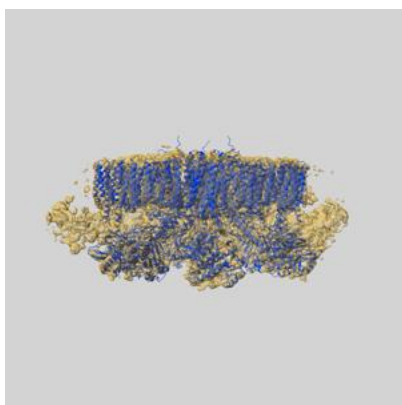
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.48	-	-
Author-provided FSC curve	4.48	6.75	4.59
Unmasked-calculated*	6.29	7.82	6.57

*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 6.29 differs from the reported value 4.48 by more than 10 %

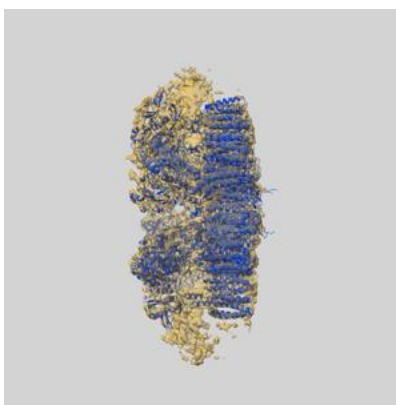
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12521 and PDB model 7NPU. Per-residue inclusion information can be found in section 3 on page 6.

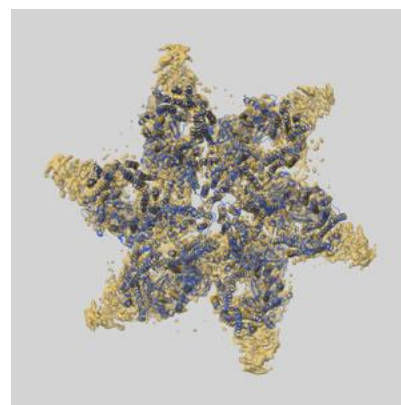
9.1 Map-model overlay [i](#)



X



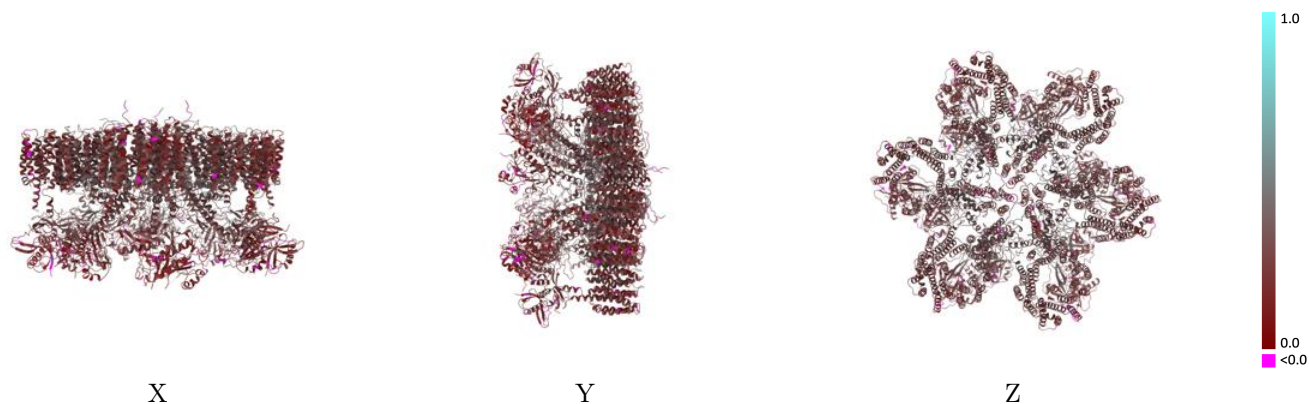
Y



Z

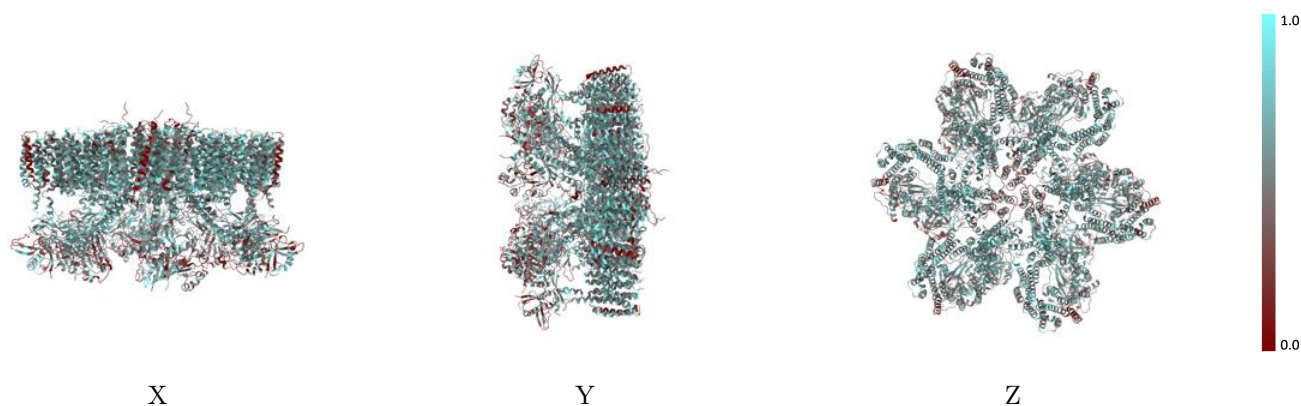
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



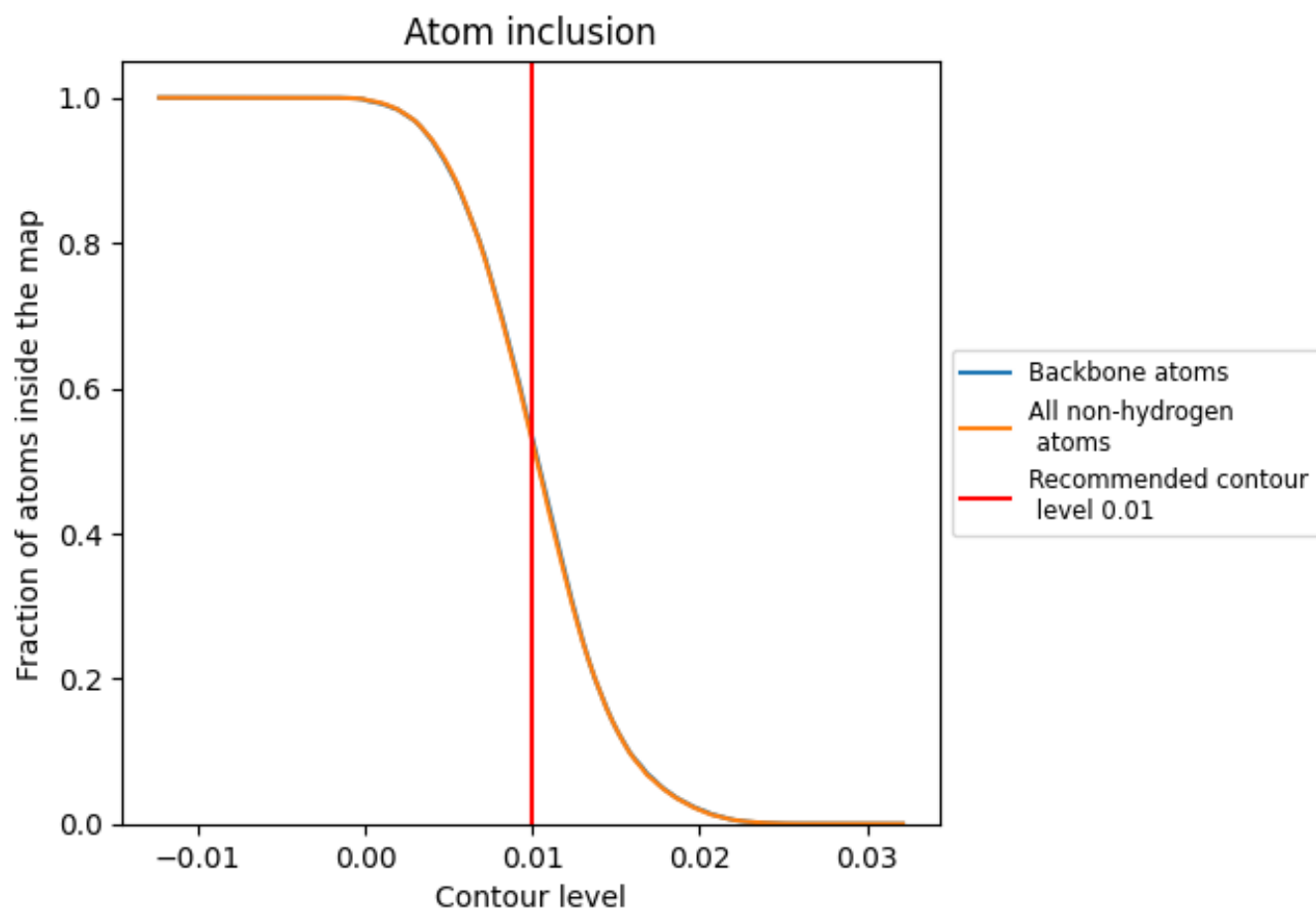
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 53% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5281	 0.2680
B1	 0.6199	 0.3350
B2	 0.6310	 0.3390
B3	 0.6384	 0.3490
B4	 0.6458	 0.3420
B5	 0.6550	 0.3440
B6	 0.6568	 0.3290
C1	 0.4811	 0.2440
C2	 0.4776	 0.2520
C3	 0.5045	 0.2590
C4	 0.4684	 0.2480
C5	 0.5227	 0.2500
C6	 0.5064	 0.2530
D1	 0.5804	 0.2840
D2	 0.5502	 0.2680
D3	 0.5782	 0.2830
D4	 0.5567	 0.2610
D5	 0.5626	 0.2800
D6	 0.5417	 0.2530
D7	 0.5384	 0.2710
D8	 0.5094	 0.2580
D9	 0.5691	 0.2840
DA	 0.5451	 0.2590
DB	 0.5618	 0.2750
DC	 0.5163	 0.2610

