



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:49 AM UTC

PDB ID : 7NP7 / pdb_00007np7
EMDB ID : EMD-12514
Title : Structure of an intact ESX-5 inner membrane complex, Composite C1 model
Authors : Fahrenkamp, D.; Bunduc, C.M.; Wald, J.; Ummels, R.; Bitter, W.; Houben, E.N.G.; Marlovits, T.C.
Deposited on : 2021-02-26
Resolution : 4.03 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

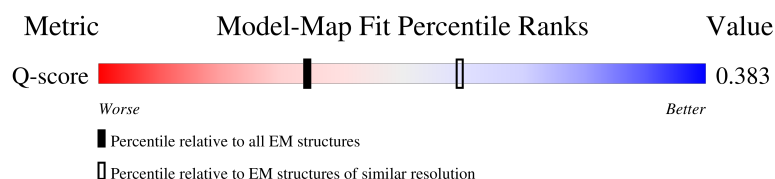
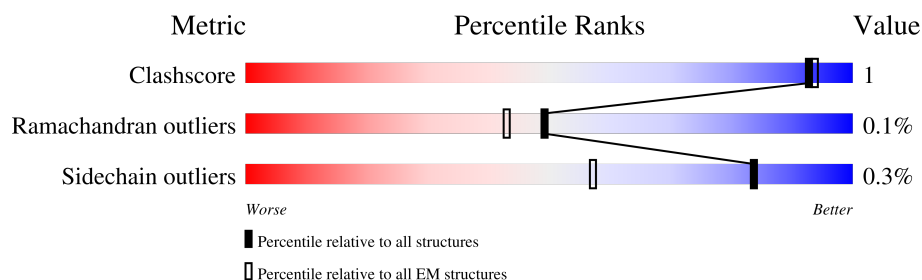
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.03 Å.

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



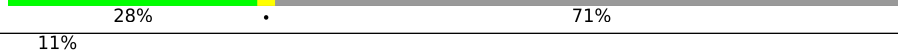
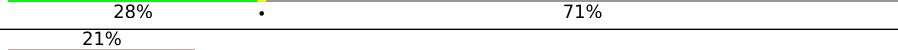
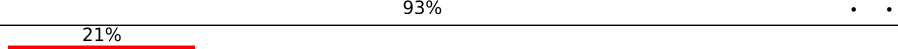
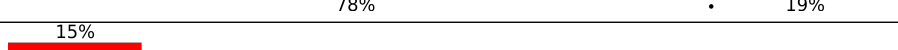
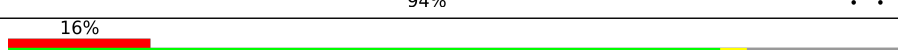
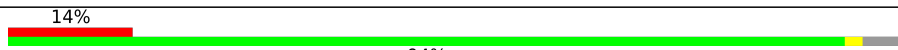
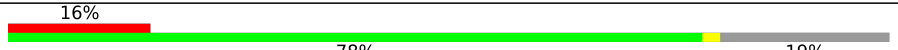
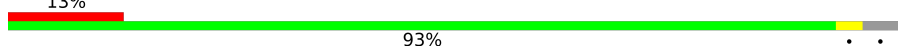
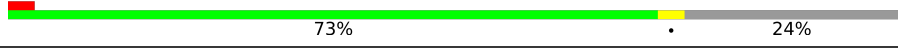
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6618 (3.54 - 4.53)

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	8% 91% 6%
1	B2	506	8% 87% 7% 6%
1	B3	506	9% 89% 6% 6%
1	B4	506	90% 5% 5%

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Mol	Chain	Length	Quality of chain
1	B5	506	
1	B6	506	
2	C1	1391	
2	C2	1391	
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	
4	P1	585	
4	P2	585	
4	P3	585	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 182470 atoms, of which 92300 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
1	B1	478	Total	C	H	N	O	S	0	0
			7218	2266	3631	639	671	11		
1	B2	478	Total	C	H	N	O	S	0	0
			7218	2266	3631	639	671	11		
1	B3	478	Total	C	H	N	O	S	0	0
			7218	2266	3631	639	671	11		
1	B4	480	Total	C	H	N	O	S	0	0
			7212	2262	3621	644	675	10		
1	B5	480	Total	C	H	N	O	S	0	0
			7212	2262	3621	644	675	10		
1	B6	480	Total	C	H	N	O	S	0	0
			7212	2262	3621	644	675	10		

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

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

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

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

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

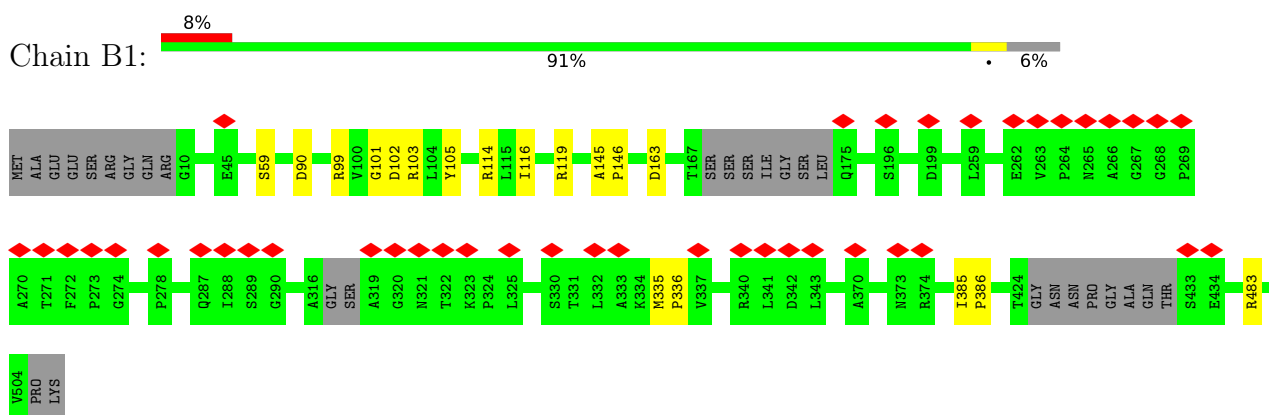
- Molecule 4 is a protein called Mycosin-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	P1	444	Total	C	H	N	O	S	0	0
			6445	2046	3219	554	611	15		
4	P2	444	Total	C	H	N	O	S	0	0
			6445	2046	3219	554	611	15		
4	P3	444	Total	C	H	N	O	S	0	0
			6445	2046	3219	554	611	15		

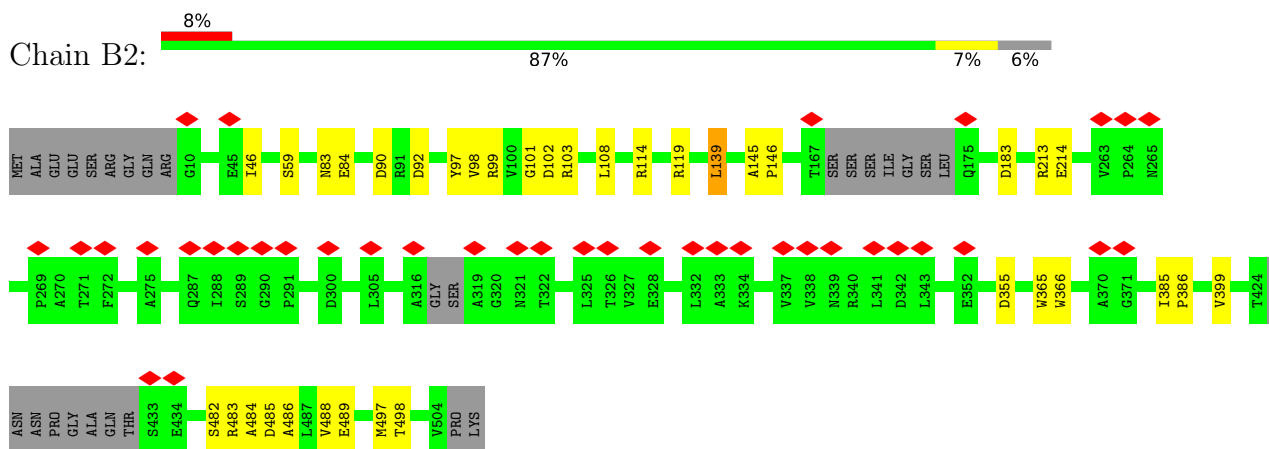
3 Residue-property plots

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.

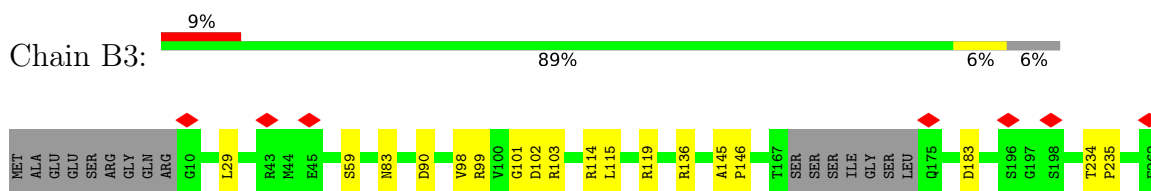
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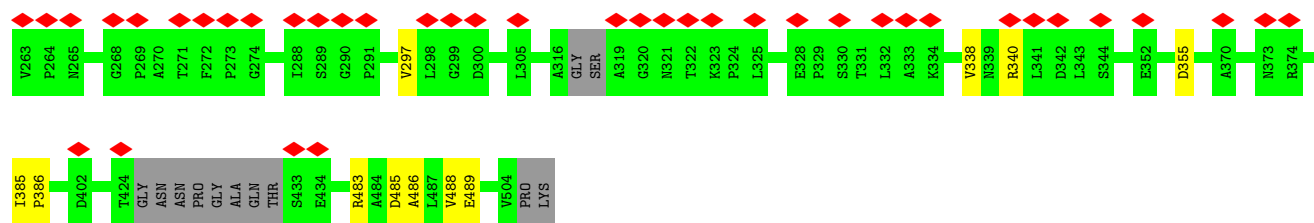


- Molecule 1: ESX-5 secretion system ATPase EccB5



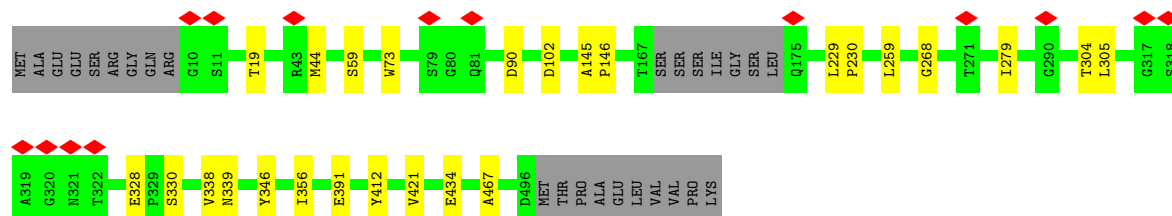
- Molecule 1: ESX-5 secretion system ATPase EccB5





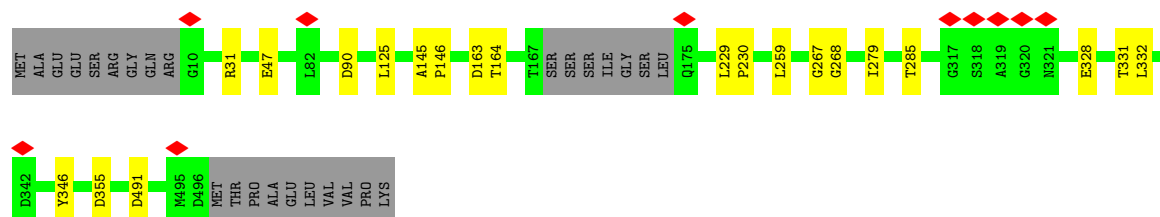
- Molecule 1: ESX-5 secretion system ATPase EccB5

Chain B4: 90% 5% 5%



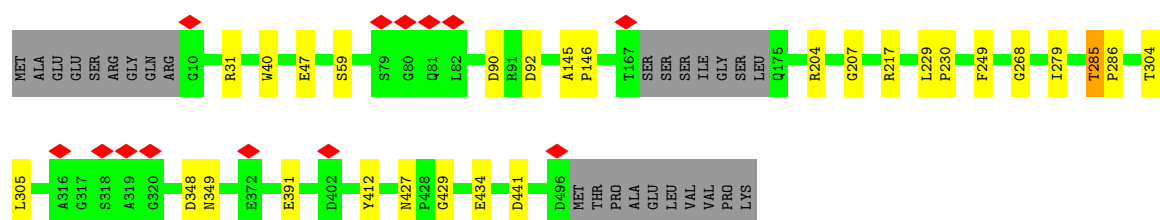
- Molecule 1: ESX-5 secretion system ATPase EccB5

Chain B5: 91% 5% 5%



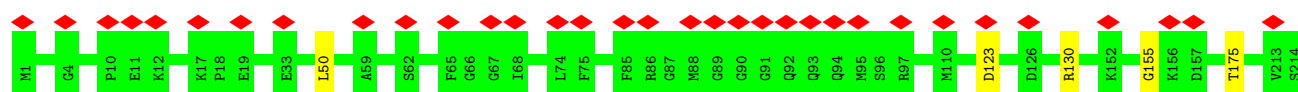
- Molecule 1: ESX-5 secretion system ATPase EccB5

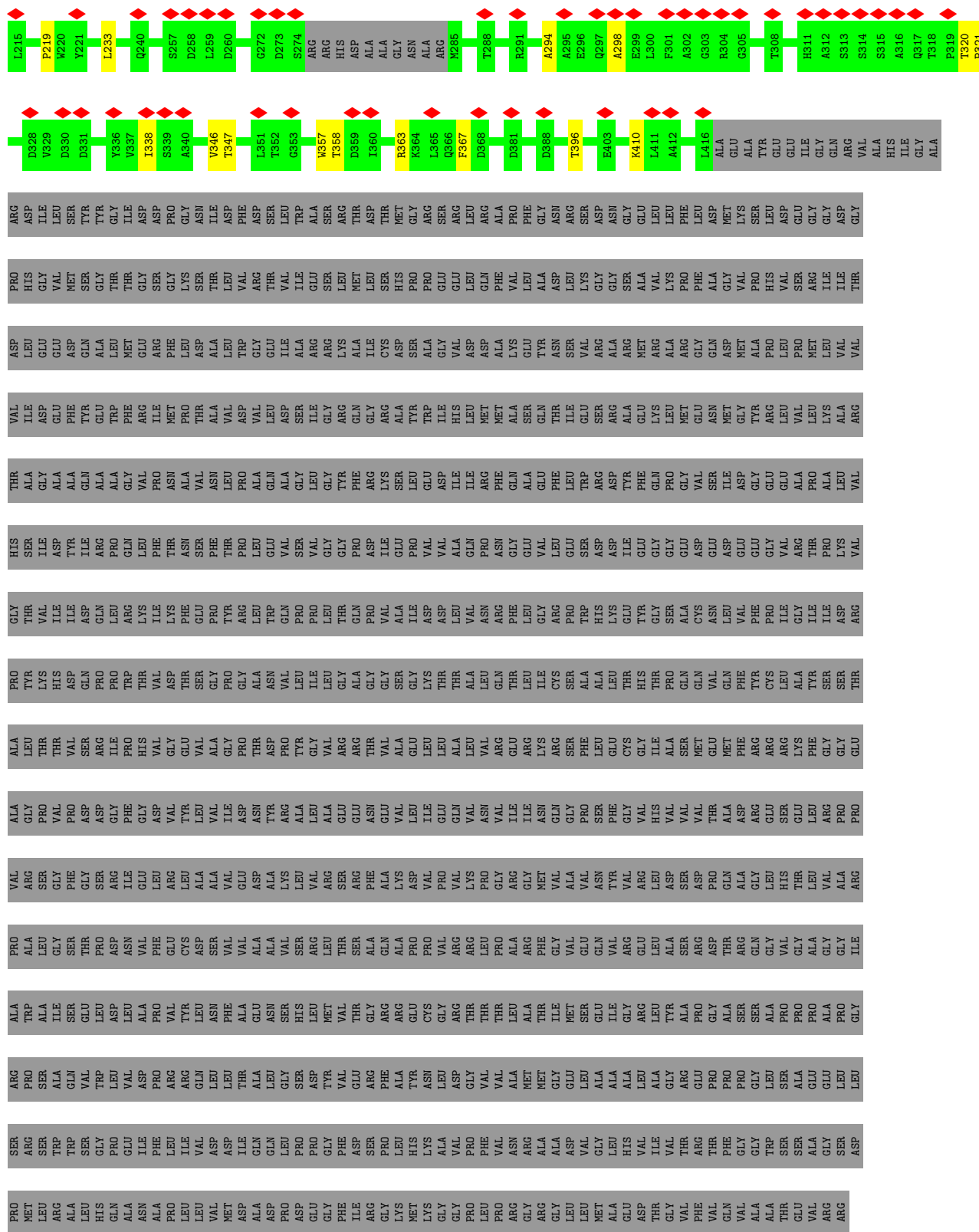
Chain B6: 89% 5% 5%



- Molecule 2: ESX-5 secretion system protein EccC5

Chain C1: 6% 28% 71%

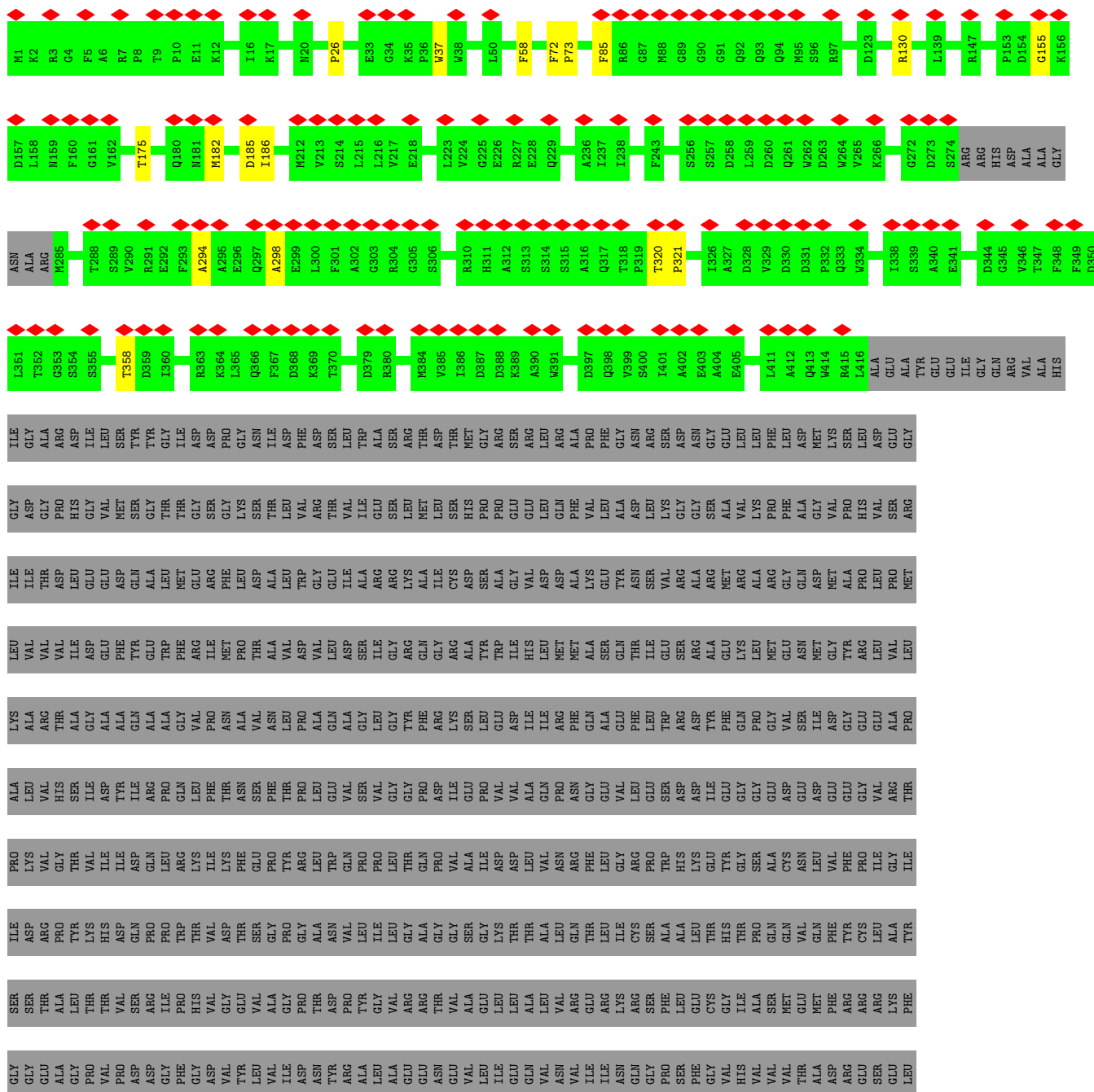




• Molecule 2: ESX-5 secretion system protein EccC5

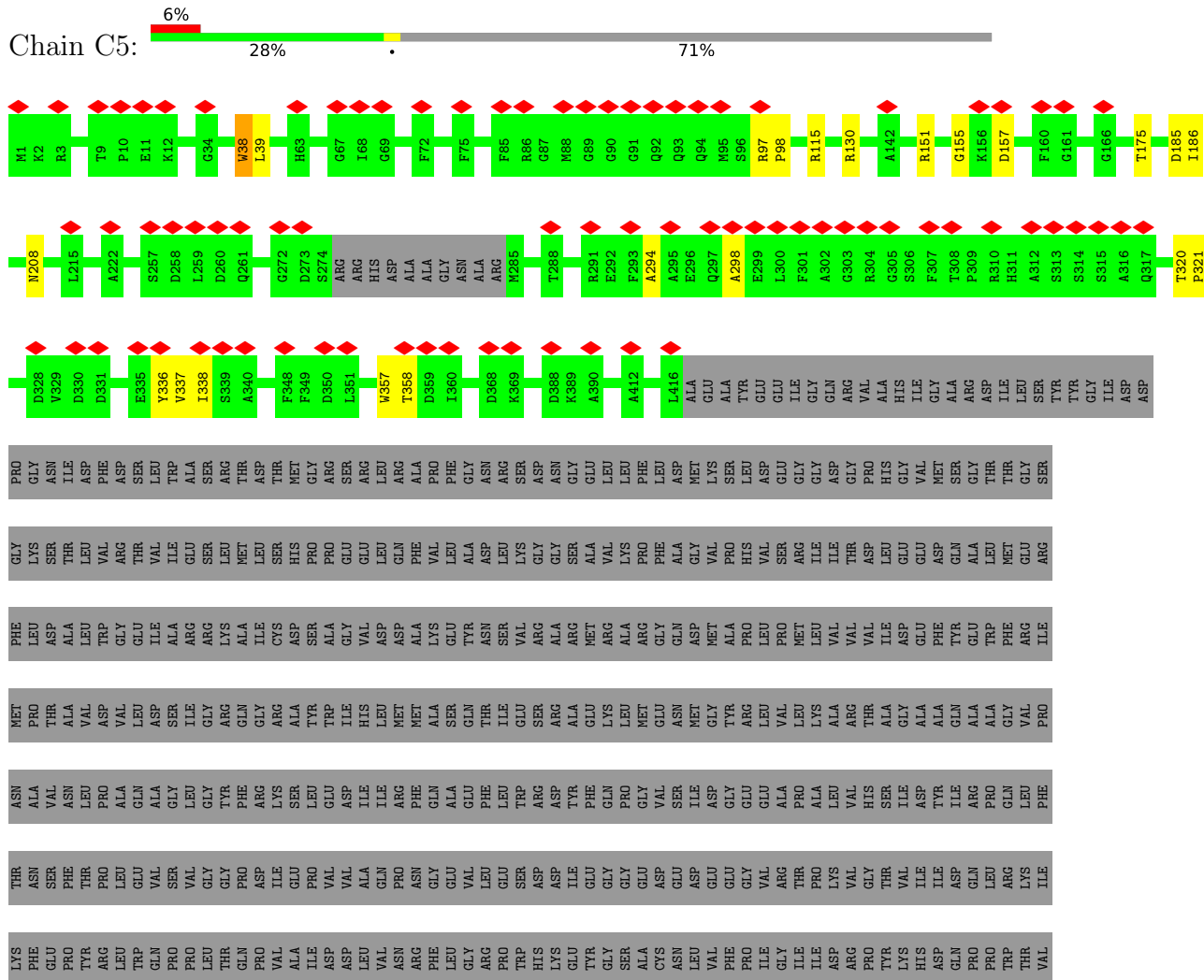






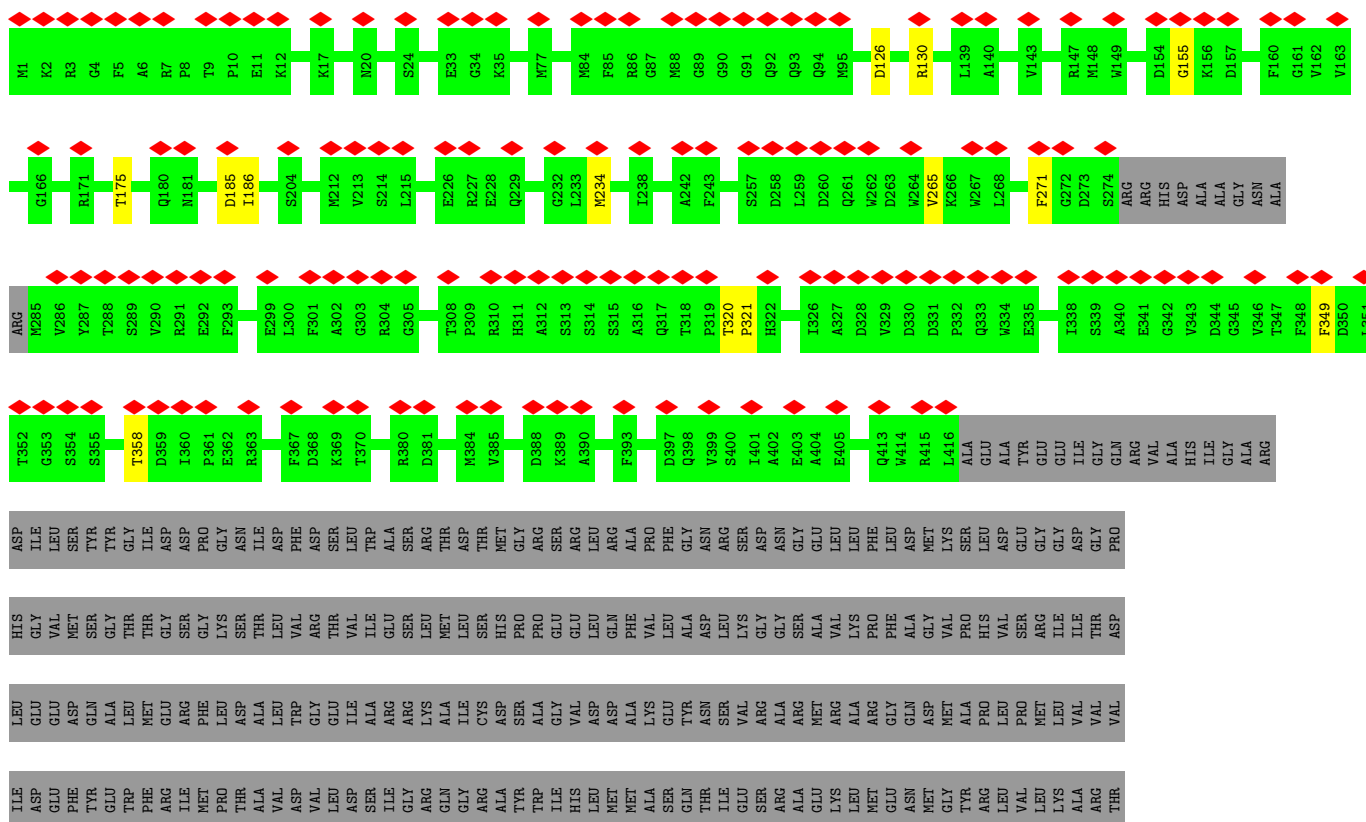
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		ASP	SER	ARG	ARG	GLY	ALA	ARG	ALA	PRO
		PRO	ARG	ARG	PRO	ARG	TRP	ALA	VAL	ARG
		LEU	SER	TRP	SER	ALA	ILE	LEU	GLY	GLY
		ALA	TRP	TRP	GLN	GLN	SER	SER	GLY	PHE
		LEU	SER	VAL	SER	VAL	GLU	THR	GLY	GLY
		HIS	GLY	TRP	TRP	TRP	LEU	PRO	SER	SER
		GLN	PRO	GLY	GLY	ASP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

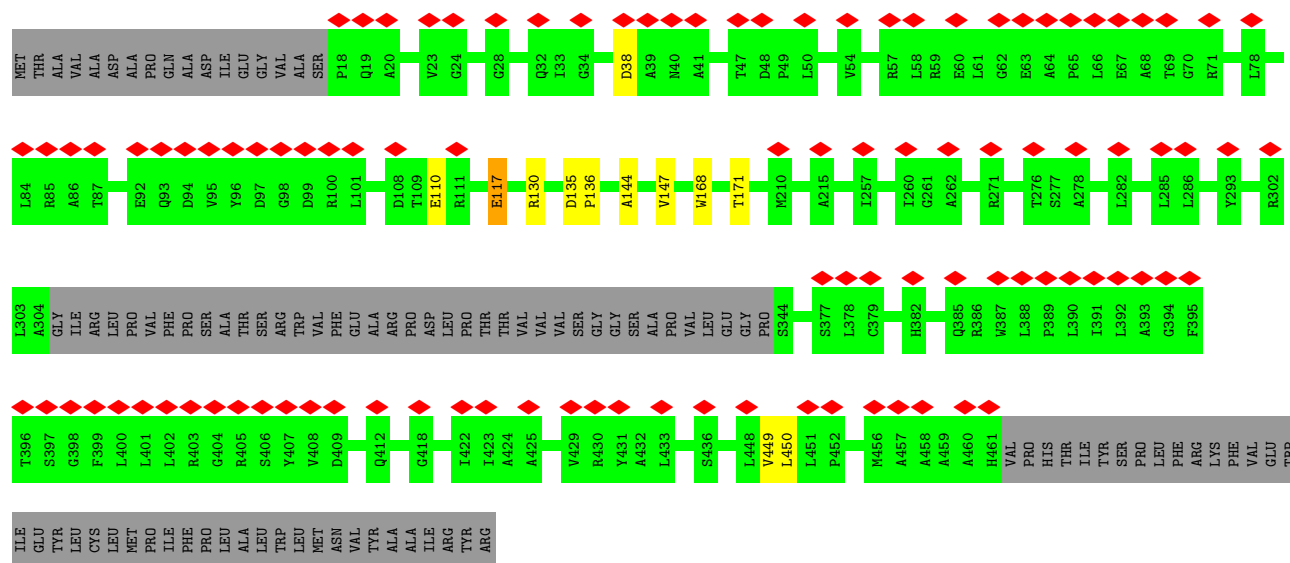
- Molecule 2: ESX-5 secretion system protein EccC5



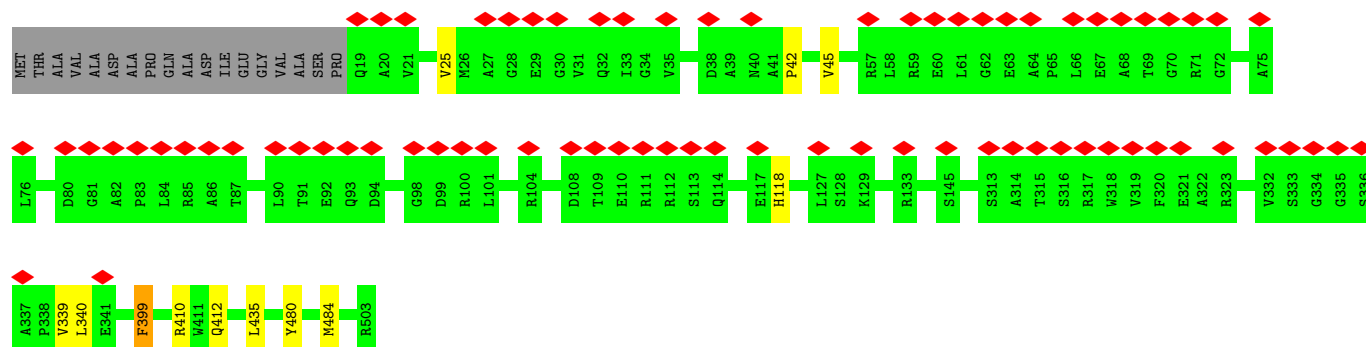
[illegible]

- Molecule 2: ESX-5 secretion system protein EccC5

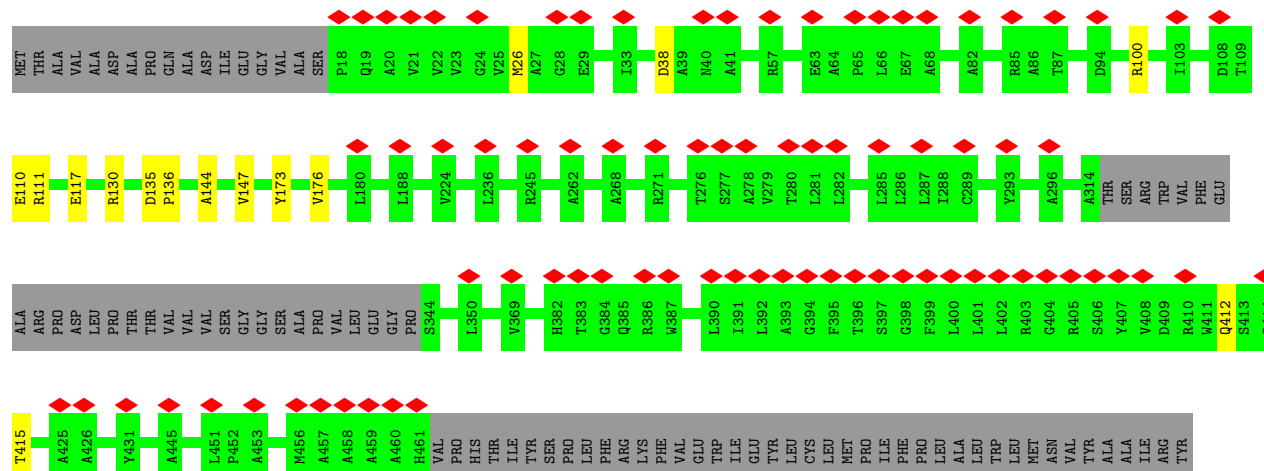
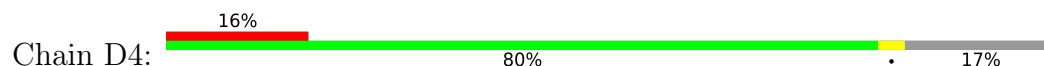


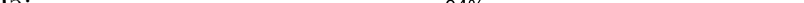


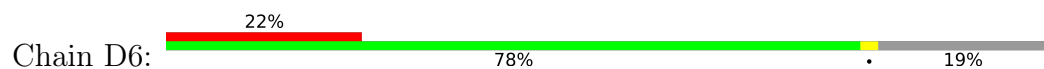
• Molecule 3: ESX-5 secretion system protein EccD5

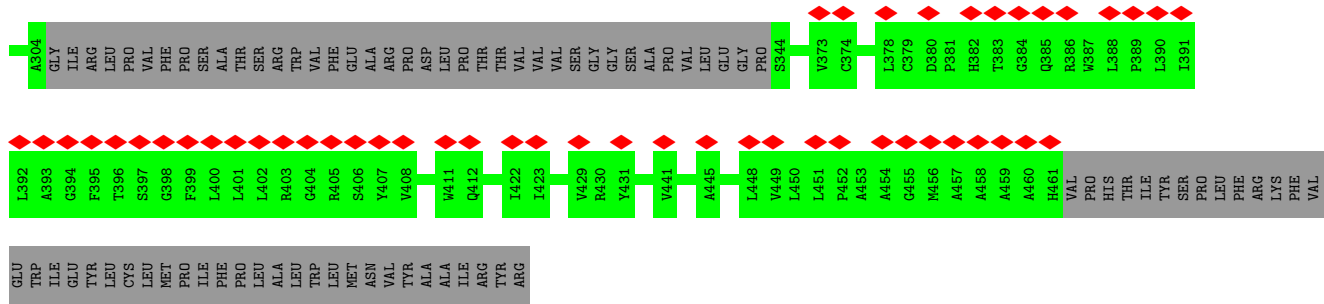


• Molecule 3: ESX-5 secretion system protein EccD5

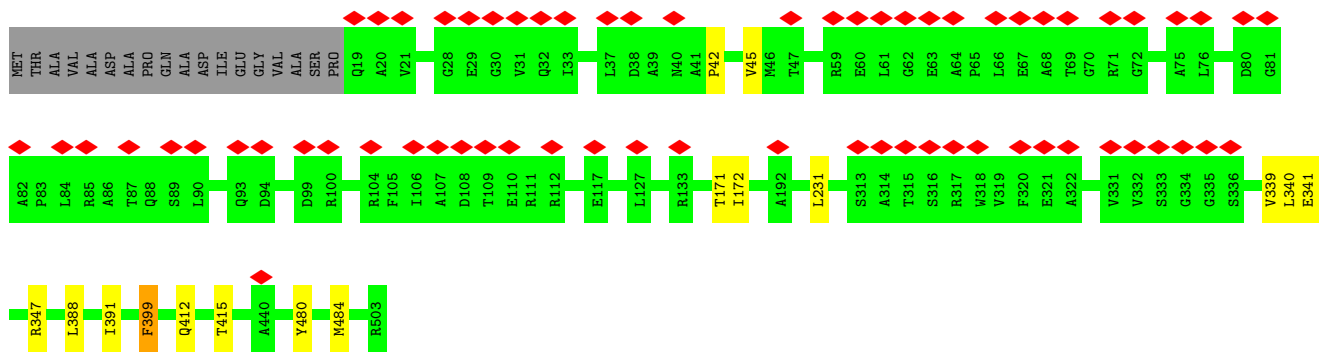


Chain D5:  21% 94%

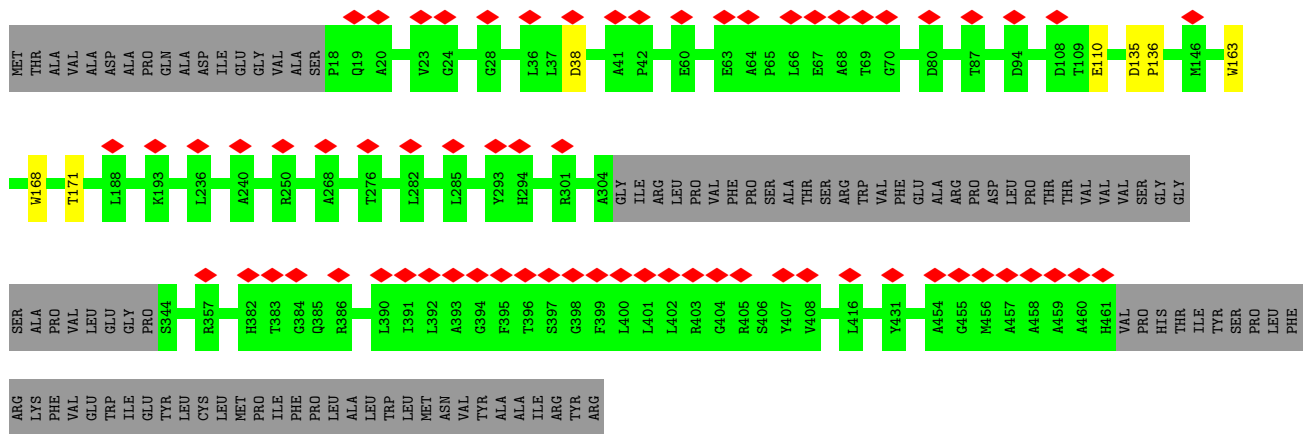
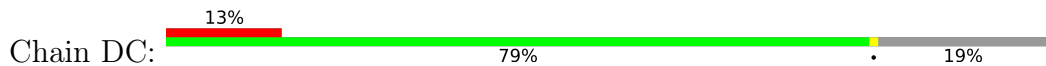




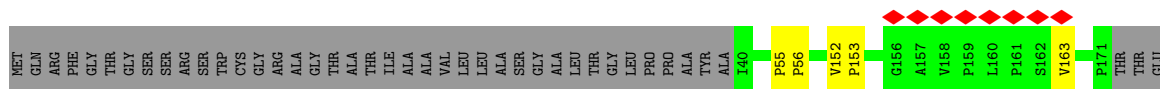
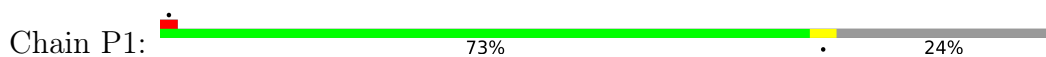
- Molecule 3: ESX-5 secretion system protein EccD5



- Molecule 3: ESX-5 secretion system protein EccD5



- Molecule 4: Mycosin-5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154929	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	0.055	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B1	0.73	13/3669 (0.4%)	0.91	15/5028 (0.3%)
1	B2	0.80	16/3669 (0.4%)	0.99	29/5028 (0.6%)
1	B3	0.78	14/3669 (0.4%)	0.98	21/5028 (0.4%)
1	B4	0.42	0/3675	0.75	1/5038 (0.0%)
1	B5	0.41	0/3675	0.80	0/5038
1	B6	0.41	0/3675	0.76	1/5038 (0.0%)
2	C1	0.33	0/3280	0.81	1/4459 (0.0%)
2	C2	0.32	0/3280	0.79	0/4459
2	C3	0.35	0/3280	0.80	2/4459 (0.0%)
2	C4	0.33	0/3280	0.79	0/4459
2	C5	0.34	0/3280	0.80	0/4459
2	C6	0.34	0/3280	0.81	0/4459
3	D1	0.35	0/3710	0.73	0/5078
3	D2	0.31	0/3038	0.73	0/4151
3	D3	0.39	0/3710	0.75	1/5078 (0.0%)
3	D4	0.32	0/3115	0.74	0/4257
3	D5	0.36	0/3710	0.73	0/5078
3	D6	0.31	0/3038	0.73	0/4151
3	D7	0.38	0/3710	0.75	0/5078
3	D8	0.32	0/3038	0.74	0/4151
3	D9	0.36	0/3710	0.73	0/5078
3	DA	0.30	0/3038	0.72	0/4151
3	DB	0.38	0/3710	0.74	0/5078
3	DC	0.31	0/3038	0.75	0/4151
4	P1	0.58	3/3309 (0.1%)	0.89	4/4545 (0.1%)
4	P2	0.58	4/3309 (0.1%)	0.90	6/4545 (0.1%)
4	P3	0.57	4/3309 (0.1%)	0.89	8/4545 (0.2%)
All	All	0.45	54/92204 (0.1%)	0.80	89/126067 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P2	0	1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B2	483	ARG	CZ-NH2	-8.61	1.22	1.33
1	B1	103	ARG	CZ-NH2	-8.41	1.22	1.33
1	B2	103	ARG	CZ-NH2	-8.31	1.22	1.33
1	B2	119	ARG	CZ-NH2	-8.30	1.22	1.33
1	B1	119	ARG	CZ-NH2	-8.27	1.22	1.33
4	P3	549	ARG	CZ-NH2	-8.21	1.22	1.33
1	B1	483	ARG	CZ-NH2	-8.14	1.22	1.33
4	P1	549	ARG	CZ-NH2	-8.08	1.23	1.33
1	B2	99	ARG	CZ-NH2	-8.02	1.23	1.33
4	P1	547	ALA	CA-CB	-8.02	1.41	1.53
1	B1	99	ARG	CZ-NH2	-8.00	1.23	1.33
1	B3	103	ARG	CZ-NH2	-7.96	1.23	1.33
4	P2	549	ARG	CZ-NH2	-7.88	1.23	1.33
1	B3	483	ARG	CZ-NH2	-7.75	1.23	1.33
1	B2	483	ARG	CZ-NH1	-7.71	1.22	1.32
1	B3	119	ARG	CZ-NH2	-7.68	1.23	1.33
4	P2	538	ALA	CA-CB	-7.66	1.43	1.54
1	B3	99	ARG	CZ-NH2	-7.64	1.23	1.33
1	B1	483	ARG	CZ-NH1	-7.34	1.22	1.32
1	B1	103	ARG	CZ-NH1	-7.32	1.22	1.32
1	B2	99	ARG	CZ-NH1	-7.29	1.22	1.32
1	B2	103	ARG	CZ-NH1	-7.20	1.22	1.32
1	B1	119	ARG	CZ-NH1	-7.12	1.22	1.32
4	P3	549	ARG	CZ-NH1	-7.07	1.22	1.32
1	B2	119	ARG	CZ-NH1	-7.06	1.22	1.32
1	B1	99	ARG	CZ-NH1	-7.04	1.22	1.32
4	P1	549	ARG	CZ-NH1	-7.03	1.23	1.32
1	B3	99	ARG	CZ-NH1	-6.96	1.23	1.32
1	B3	483	ARG	CZ-NH1	-6.95	1.23	1.32
1	B3	103	ARG	CZ-NH1	-6.82	1.23	1.32
4	P2	549	ARG	CZ-NH1	-6.70	1.23	1.32
1	B3	486	ALA	CA-CB	-6.48	1.42	1.53
1	B2	486	ALA	CA-CB	-6.41	1.42	1.53
1	B3	119	ARG	CZ-NH1	-6.35	1.23	1.32
1	B2	101	GLY	N-CA	-6.33	1.36	1.45
4	P3	547	ALA	CA-CB	-6.24	1.42	1.53
1	B2	484	ALA	CA-CB	-6.22	1.43	1.53
1	B2	99	ARG	CD-NE	-5.85	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B3	101	GLY	N-CA	-5.76	1.37	1.45
1	B3	103	ARG	CD-NE	-5.60	1.38	1.46
1	B1	483	ARG	CD-NE	-5.52	1.38	1.46
1	B1	103	ARG	CD-NE	-5.50	1.38	1.46
1	B1	119	ARG	CD-NE	-5.42	1.38	1.46
1	B2	483	ARG	CD-NE	-5.42	1.38	1.46
4	P2	549	ARG	CD-NE	-5.41	1.38	1.46
1	B3	99	ARG	CD-NE	-5.34	1.38	1.46
1	B3	483	ARG	CD-NE	-5.21	1.39	1.46
1	B2	119	ARG	CD-NE	-5.21	1.39	1.46
1	B3	119	ARG	CD-NE	-5.20	1.39	1.46
1	B1	99	ARG	CD-NE	-5.11	1.39	1.46
1	B2	102	ASP	CA-CB	-5.09	1.46	1.53
1	B1	102	ASP	CA-CB	-5.06	1.46	1.53
4	P3	549	ARG	CD-NE	-5.04	1.39	1.46
1	B2	103	ARG	CD-NE	-5.02	1.39	1.46

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B1	114	ARG	CA-C-N	7.70	130.59	120.28
1	B1	114	ARG	C-N-CA	7.70	130.59	120.28
1	B1	103	ARG	CA-CB-CG	7.54	129.18	114.10
1	B2	114	ARG	CA-C-N	7.31	130.07	120.28
1	B2	114	ARG	C-N-CA	7.31	130.07	120.28
1	B2	103	ARG	CA-CB-CG	7.15	128.40	114.10
1	B3	488	VAL	CA-C-N	7.11	133.23	122.93
1	B3	488	VAL	C-N-CA	7.11	133.23	122.93
1	B3	114	ARG	CA-C-N	6.88	129.50	120.28
1	B3	114	ARG	C-N-CA	6.88	129.50	120.28
4	P2	550	ASP	CA-CB-CG	6.80	119.40	112.60
1	B3	103	ARG	CA-CB-CG	6.72	127.55	114.10
1	B2	488	VAL	CA-C-N	6.69	133.63	122.87
1	B2	488	VAL	C-N-CA	6.69	133.63	122.87
4	P2	539	PRO	CA-C-N	6.67	131.04	121.50
4	P2	539	PRO	C-N-CA	6.67	131.04	121.50
4	P1	539	PRO	CA-C-N	6.48	131.12	121.72
4	P1	539	PRO	C-N-CA	6.48	131.12	121.72
4	P3	549	ARG	CD-NE-CZ	6.44	133.42	124.40
1	B3	489	GLU	CA-CB-CG	6.42	126.94	114.10
4	P3	549	ARG	CA-CB-CG	6.41	126.93	114.10
1	B2	98	VAL	CA-C-N	6.39	131.28	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B2	98	VAL	C-N-CA	6.39	131.28	122.77
4	P3	548	PRO	CA-C-N	6.39	129.79	120.71
4	P3	548	PRO	C-N-CA	6.39	129.79	120.71
4	P3	539	PRO	CA-C-N	6.35	130.88	122.30
4	P3	539	PRO	C-N-CA	6.35	130.88	122.30
1	B2	101	GLY	CA-C-N	6.23	132.27	122.49
1	B2	101	GLY	C-N-CA	6.23	132.27	122.49
1	B2	99	ARG	CA-CB-CG	6.12	126.33	114.10
1	B1	99	ARG	CD-NE-CZ	5.87	132.62	124.40
1	B2	489	GLU	CA-CB-CG	5.85	125.79	114.10
4	P2	549	ARG	CA-C-N	5.80	129.60	121.02
4	P2	549	ARG	C-N-CA	5.80	129.60	121.02
1	B1	119	ARG	CD-NE-CZ	5.78	132.49	124.40
4	P1	549	ARG	CD-NE-CZ	5.69	132.36	124.40
1	B2	119	ARG	CA-CB-CG	5.68	125.46	114.10
1	B3	483	ARG	N-CA-CB	5.67	118.56	110.06
1	B2	119	ARG	CD-NE-CZ	5.65	132.31	124.40
1	B1	105	TYR	CA-CB-CG	5.62	124.02	113.90
1	B1	99	ARG	CA-C-N	5.60	131.26	122.70
1	B1	99	ARG	C-N-CA	5.60	131.26	122.70
1	B3	102	ASP	CA-C-N	5.58	131.31	122.94
1	B3	102	ASP	C-N-CA	5.58	131.31	122.94
1	B3	83	ASN	CA-C-N	5.56	128.29	120.28
1	B3	83	ASN	C-N-CA	5.56	128.29	120.28
1	B3	115	LEU	CA-C-N	5.55	127.67	120.56
1	B3	115	LEU	C-N-CA	5.55	127.67	120.56
1	B3	119	ARG	CD-NE-CZ	5.54	132.16	124.40
1	B4	434	GLU	N-CA-C	5.53	120.15	112.90
1	B2	119	ARG	CG-CD-NE	5.48	124.06	112.00
1	B3	99	ARG	CD-NE-CZ	5.47	132.05	124.40
1	B2	485	ASP	CA-C-N	5.46	128.62	120.31
1	B2	485	ASP	C-N-CA	5.46	128.62	120.31
1	B3	99	ARG	CA-C-N	5.42	130.59	123.11
1	B3	99	ARG	C-N-CA	5.42	130.59	123.11
2	C3	34	GLY	CA-C-N	5.32	128.04	120.49
2	C3	34	GLY	C-N-CA	5.32	128.04	120.49
1	B1	116	ILE	CA-C-N	5.31	127.83	120.29
1	B1	116	ILE	C-N-CA	5.31	127.83	120.29
4	P1	549	ARG	CA-CB-CG	5.30	124.71	114.10
1	B2	139	LEU	CA-C-N	5.30	131.11	122.69
1	B2	139	LEU	C-N-CA	5.30	131.11	122.69
2	C1	396	THR	N-CA-C	5.27	118.08	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B1	101	GLY	CA-C-N	5.26	131.04	122.67
1	B1	101	GLY	C-N-CA	5.26	131.04	122.67
4	P3	546	PRO	CA-C-N	5.26	127.96	120.49
4	P3	546	PRO	C-N-CA	5.26	127.96	120.49
1	B2	483	ARG	CA-C-N	5.25	128.29	120.31
1	B2	483	ARG	C-N-CA	5.25	128.29	120.31
1	B3	486	ALA	CA-C-N	5.22	131.51	121.54
1	B3	486	ALA	C-N-CA	5.22	131.51	121.54
3	D3	118	HIS	N-CA-C	5.21	117.46	109.07
1	B3	98	VAL	CA-C-N	5.18	129.49	122.19
1	B3	98	VAL	C-N-CA	5.18	129.49	122.19
4	P2	549	ARG	CA-CB-CG	5.17	124.43	114.10
1	B6	434	GLU	N-CA-C	5.16	119.67	112.90
1	B1	483	ARG	N-CA-CB	5.16	118.17	110.22
1	B2	102	ASP	CA-C-N	5.16	131.09	122.73
1	B2	102	ASP	C-N-CA	5.16	131.09	122.73
1	B1	119	ARG	CG-CD-NE	5.15	123.34	112.00
1	B2	483	ARG	N-CA-CB	5.13	118.24	110.14
1	B2	97	TYR	CA-C-N	5.11	130.12	123.06
1	B2	97	TYR	C-N-CA	5.11	130.12	123.06
1	B2	99	ARG	CG-CD-NE	5.11	123.23	112.00
1	B1	119	ARG	CA-CB-CG	5.10	124.30	114.10
1	B2	482	SER	CA-C-N	5.04	127.74	120.38
1	B2	482	SER	C-N-CA	5.04	127.74	120.38
1	B2	483	ARG	CB-CG-CD	5.04	122.89	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	P2	444	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	3587	3631	3626	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B2	3587	3631	3626	16	0
1	B3	3587	3631	3626	11	0
1	B4	3591	3621	3618	17	0
1	B5	3591	3621	3618	11	0
1	B6	3591	3621	3618	16	0
2	C1	3190	3145	3142	13	0
2	C2	3190	3145	3142	9	0
2	C3	3190	3145	3142	10	0
2	C4	3190	3145	3142	10	0
2	C5	3190	3145	3142	13	0
2	C6	3190	3145	3142	10	0
3	D1	3635	3823	3822	13	0
3	D2	2989	3166	3163	8	0
3	D3	3635	3824	3822	7	0
3	D4	3063	3245	3243	9	0
3	D5	3635	3824	3822	6	0
3	D6	2989	3166	3163	6	0
3	D7	3635	3824	3822	8	0
3	D8	2989	3165	3163	9	0
3	D9	3635	3824	3822	13	0
3	DA	2989	3167	3163	5	0
3	DB	3635	3824	3822	11	0
3	DC	2989	3165	3163	4	0
4	P1	3226	3219	3218	9	0
4	P2	3226	3219	3218	7	0
4	P3	3226	3219	3218	13	0
All	All	90170	92300	92228	250	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.

All (250) 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:C4:130:ARG:NH2	3:DA:110:GLU:OE2	2.22	0.72
2:C1:130:ARG:NH2	3:D8:110:GLU:OE2	2.22	0.72
2:C2:130:ARG:NH2	3:D6:110:GLU:OE2	2.25	0.70
2:C3:130:ARG:NH2	3:DC:110:GLU:OE2	2.26	0.69
4:P1:552:VAL:HG23	4:P1:553:PRO:HD3	1.75	0.69
2:C5:185:ASP:OD1	2:C5:186:ILE:N	2.26	0.68
2:C4:185:ASP:OD1	2:C4:186:ILE:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D6:432:ALA:HB2	3:D6:444:VAL:HG21	1.83	0.61
1:B6:391:GLU:OE2	1:B6:412:TYR:OH	2.19	0.60
3:D9:412:GLN:O	3:D9:415:THR:HG22	2.03	0.59
1:B5:31:ARG:NH1	1:B5:47:GLU:OE1	2.35	0.58
1:B2:355:ASP:OD1	1:B2:355:ASP:N	2.37	0.57
3:DB:341:GLU:OE2	3:DB:347:ARG:NE	2.26	0.57
2:C5:130:ARG:NH2	3:D4:110:GLU:OE2	2.38	0.56
3:D8:380:ASP:OD2	3:D8:430:ARG:NH2	2.39	0.55
2:C6:130:ARG:NH2	3:D2:110:GLU:OE2	2.40	0.55
3:D1:311:PHE:CG	3:D1:312:PRO:HD2	2.42	0.55
1:B5:328:GLU:O	1:B5:331:THR:HG22	2.05	0.55
1:B6:31:ARG:NH1	1:B6:47:GLU:OE1	2.34	0.55
1:B4:259:LEU:O	1:B4:346:TYR:OH	2.22	0.54
1:B1:385:ILE:HG23	1:B1:386:PRO:HD2	1.90	0.53
2:C3:358:THR:HG22	2:C3:358:THR:O	2.08	0.53
1:B5:268:GLY:O	1:B5:279:ILE:HG22	2.09	0.53
2:C5:358:THR:HG22	2:C5:358:THR:O	2.09	0.53
3:D4:26:MET:HE3	3:D4:100:ARG:HD2	1.91	0.53
1:B5:163:ASP:OD2	1:B5:164:THR:N	2.42	0.52
2:C2:320:THR:CG2	2:C2:321:PRO:HD3	2.40	0.52
2:C6:185:ASP:OD1	2:C6:186:ILE:N	2.43	0.52
3:DA:135:ASP:HB2	3:DA:136:PRO:HD2	1.91	0.52
2:C3:320:THR:CG2	2:C3:321:PRO:HD3	2.39	0.51
2:C4:358:THR:O	2:C4:358:THR:HG22	2.09	0.51
2:C4:320:THR:CG2	2:C4:321:PRO:HD3	2.40	0.51
1:B6:427:ASN:OD1	1:B6:429:GLY:N	2.41	0.51
3:D1:484:MET:HB3	3:D1:485:PRO:HD3	1.93	0.51
3:DB:231:LEU:HD11	4:P3:557:ALA:HA	1.92	0.51
1:B2:213:ARG:NE	1:B2:214:GLU:OE2	2.43	0.51
2:C5:294:ALA:HA	2:C5:298:ALA:HB3	1.93	0.51
4:P3:552:VAL:HG23	4:P3:553:PRO:HD3	1.92	0.51
2:C1:358:THR:HG22	2:C1:358:THR:O	2.11	0.50
2:C1:320:THR:CG2	2:C1:321:PRO:HD3	2.42	0.50
3:D8:135:ASP:HB2	3:D8:136:PRO:HD2	1.93	0.50
2:C6:320:THR:CG2	2:C6:321:PRO:HD3	2.41	0.50
2:C5:320:THR:CG2	2:C5:321:PRO:HD3	2.41	0.50
3:D5:311:PHE:CG	3:D5:312:PRO:HD2	2.47	0.50
4:P1:442:SER:HB2	4:P1:449:ILE:HG23	1.93	0.50
4:P2:148:MET:HE1	4:P2:438:VAL:HG13	1.92	0.50
3:D7:412:GLN:O	3:D7:415:THR:HG22	2.12	0.50
3:D8:206:MET:HE1	3:D8:253:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D1:399:PHE:CD1	3:D1:399:PHE:C	2.90	0.50
1:B1:59:SER:OG	3:DB:484:MET:HA	2.12	0.49
1:B2:385:ILE:HG23	1:B2:386:PRO:HD2	1.94	0.49
2:C3:294:ALA:HA	2:C3:298:ALA:HB3	1.94	0.49
2:C3:338:ILE:HD11	2:C3:357:TRP:CH2	2.47	0.49
3:D9:311:PHE:CG	3:D9:312:PRO:HD2	2.46	0.49
3:D5:151:VAL:O	3:D5:155:THR:HG23	2.13	0.49
1:B3:385:ILE:HG23	1:B3:386:PRO:HD2	1.95	0.49
2:C6:265:VAL:HG13	2:C6:271:PHE:CD1	2.47	0.49
1:B3:355:ASP:N	1:B3:355:ASP:OD1	2.43	0.49
1:B1:163:ASP:C	1:B1:163:ASP:OD2	2.56	0.48
1:B4:328:GLU:OE2	1:B4:330:SER:N	2.45	0.48
3:D1:25:VAL:N	3:D1:33:ILE:O	2.46	0.48
2:C5:97:ARG:HB3	2:C5:98:PRO:HD3	1.95	0.48
2:C2:185:ASP:OD1	2:C2:186:ILE:N	2.46	0.48
2:C2:358:THR:HG22	2:C2:358:THR:O	2.13	0.48
3:D1:354:GLU:OE1	3:D2:130:ARG:NH1	2.46	0.48
1:B6:145:ALA:HB1	1:B6:146:PRO:HD2	1.96	0.48
2:C6:358:THR:HG22	2:C6:358:THR:O	2.14	0.48
2:C1:50:LEU:HB2	2:C2:76:MET:HE1	1.96	0.47
1:B2:145:ALA:HB1	1:B2:146:PRO:HD2	1.96	0.47
4:P2:152:VAL:HG13	4:P2:153:PRO:HD2	1.97	0.47
1:B4:391:GLU:OE2	1:B4:412:TYR:OH	2.33	0.47
1:B3:145:ALA:HB1	1:B3:146:PRO:HD2	1.97	0.47
1:B4:304:THR:HG22	1:B4:305:LEU:N	2.29	0.47
3:D7:399:PHE:CD1	3:D7:399:PHE:C	2.91	0.47
2:C1:123:ASP:OD1	3:D8:112:ARG:NE	2.42	0.46
2:C3:29:ILE:HG22	2:C3:187:GLU:HG3	1.98	0.46
2:C5:115:ARG:NH1	3:D4:117:GLU:OE1	2.48	0.46
2:C5:338:ILE:HD11	2:C5:357:TRP:CH2	2.50	0.46
3:D1:502:TYR:O	3:D1:503:ARG:C	2.58	0.46
3:D4:135:ASP:HB2	3:D4:136:PRO:HD2	1.96	0.46
2:C4:294:ALA:HA	2:C4:298:ALA:HB3	1.97	0.46
3:D6:144:ALA:O	3:D6:147:VAL:HG12	2.15	0.46
3:D7:42:PRO:O	3:D7:45:VAL:HG22	2.14	0.46
3:D9:399:PHE:CD1	3:D9:399:PHE:C	2.92	0.46
3:DB:480:TYR:CD1	3:DB:480:TYR:N	2.81	0.46
3:D7:480:TYR:CD1	3:D7:480:TYR:N	2.80	0.46
3:D2:135:ASP:HB2	3:D2:136:PRO:HD2	1.98	0.46
1:B5:355:ASP:OD1	1:B5:355:ASP:N	2.39	0.46
4:P2:163:VAL:O	4:P2:163:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:183:ASP:OD1	1:B3:183:ASP:C	2.58	0.46
3:D5:412:GLN:O	3:D5:415:THR:HG22	2.16	0.46
3:DB:412:GLN:O	3:DB:415:THR:HG22	2.16	0.46
4:P3:163:VAL:HG13	4:P3:163:VAL:O	2.16	0.46
2:C2:320:THR:HG23	2:C2:321:PRO:HD3	1.98	0.46
4:P3:442:SER:HB2	4:P3:449:ILE:HG23	1.96	0.45
2:C1:233:LEU:HD22	2:C1:367:PHE:HZ	1.81	0.45
4:P1:552:VAL:HG23	4:P1:553:PRO:CD	2.43	0.45
4:P2:552:VAL:CG2	4:P2:553:PRO:HD3	2.47	0.45
3:D9:25:VAL:N	3:D9:33:ILE:O	2.47	0.45
1:B6:304:THR:HG22	1:B6:305:LEU:N	2.31	0.45
3:D3:42:PRO:O	3:D3:45:VAL:HG22	2.17	0.45
1:B4:268:GLY:O	1:B4:279:ILE:HG22	2.17	0.45
3:D5:42:PRO:O	3:D5:45:VAL:HG22	2.16	0.45
3:D7:149:THR:O	3:D7:152:VAL:HG22	2.17	0.45
3:DA:38:ASP:OD2	3:DA:38:ASP:C	2.59	0.45
4:P1:163:VAL:O	4:P1:163:VAL:HG13	2.17	0.45
3:DB:340:LEU:HD12	3:DB:340:LEU:O	2.17	0.45
1:B3:485:ASP:C	1:B3:485:ASP:OD1	2.60	0.45
1:B4:145:ALA:HB1	1:B4:146:PRO:HD2	1.98	0.45
1:B1:145:ALA:HB1	1:B1:146:PRO:HD2	1.99	0.44
1:B2:83:ASN:CG	1:B2:84:GLU:H	2.25	0.44
1:B5:259:LEU:O	1:B5:346:TYR:OH	2.30	0.44
2:C4:72:PHE:HB2	2:C4:73:PRO:HD3	2.00	0.44
3:D1:412:GLN:O	3:D1:415:THR:HG22	2.17	0.44
3:D6:38:ASP:OD2	3:D6:38:ASP:C	2.60	0.44
1:B2:183:ASP:OD2	1:B2:183:ASP:C	2.60	0.44
2:C1:294:ALA:HA	2:C1:298:ALA:HB3	1.98	0.44
1:B6:204:ARG:NH1	1:B6:207:GLY:O	2.50	0.44
1:B6:348:ASP:OD1	1:B6:349:ASN:ND2	2.41	0.44
2:C4:26:PRO:HD2	2:C4:182:MET:SD	2.57	0.44
3:D1:42:PRO:O	3:D1:45:VAL:HG22	2.17	0.44
3:D3:339:VAL:HG12	3:D3:340:LEU:N	2.32	0.44
3:D9:40:ASN:HA	3:D9:89:SER:HB3	2.00	0.44
3:DB:388:LEU:O	3:DB:391:ILE:HG22	2.18	0.44
4:P1:152:VAL:HG13	4:P1:153:PRO:HD2	1.98	0.44
1:B4:102:ASP:OD1	1:B4:102:ASP:N	2.51	0.44
2:C4:320:THR:HG23	2:C4:321:PRO:HD3	2.00	0.44
3:D2:117:GLU:CD	3:D2:117:GLU:H	2.25	0.44
4:P2:109:ASP:CG	4:P2:110:THR:H	2.25	0.44
1:B3:136:ARG:NH1	1:B6:441:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C5:208:ASN:ND2	3:D4:111:ARG:O	2.46	0.44
3:D3:399:PHE:CD1	3:D3:399:PHE:C	2.95	0.44
3:D4:144:ALA:O	3:D4:147:VAL:HG12	2.18	0.44
4:P3:152:VAL:HG13	4:P3:153:PRO:HD2	1.98	0.44
4:P3:552:VAL:CG2	4:P3:553:PRO:HD3	2.48	0.44
3:D2:449:VAL:HG13	3:D2:450:LEU:HD12	2.00	0.44
3:D8:206:MET:HE1	3:D8:253:ILE:CD1	2.48	0.44
4:P1:299:ASP:C	4:P1:299:ASP:OD1	2.61	0.44
1:B6:90:ASP:C	1:B6:90:ASP:OD1	2.61	0.44
3:D9:42:PRO:O	3:D9:45:VAL:HG22	2.18	0.44
3:D4:38:ASP:OD2	3:D4:38:ASP:C	2.61	0.43
1:B2:108:LEU:HD21	1:B2:139:LEU:HD23	1.99	0.43
2:C1:410:LYS:HE3	3:D8:48:ASP:CG	2.43	0.43
2:C5:151:ARG:HD3	2:C5:157:ASP:OD1	2.18	0.43
3:DC:38:ASP:OD2	3:DC:38:ASP:C	2.62	0.43
3:D2:168:TRP:O	3:D2:171:THR:HG22	2.19	0.43
1:B3:338:VAL:HG12	1:B3:340:ARG:H	1.83	0.43
1:B6:217:ARG:CZ	1:B6:249:PHE:CE1	3.02	0.43
2:C3:175:THR:HG23	2:C3:175:THR:O	2.19	0.43
2:C3:233:LEU:HD22	2:C3:367:PHE:HZ	1.84	0.43
2:C1:219:PRO:HD2	2:C1:363:ARG:NH1	2.34	0.43
1:B2:59:SER:OG	3:D7:484:MET:HA	2.19	0.43
1:B3:297:VAL:O	1:B3:297:VAL:HG13	2.18	0.43
2:C6:175:THR:HG23	2:C6:175:THR:O	2.18	0.43
3:D2:38:ASP:C	3:D2:38:ASP:OD2	2.61	0.43
3:D4:412:GLN:O	3:D4:415:THR:HG22	2.18	0.43
1:B4:229:LEU:HB3	1:B4:230:PRO:HD3	2.01	0.43
1:B6:268:GLY:N	1:B6:279:ILE:HG22	2.34	0.43
4:P3:413:ASP:OD2	4:P3:413:ASP:C	2.61	0.43
4:P3:445:ASP:CG	4:P3:446:ASP:H	2.27	0.43
1:B6:59:SER:OG	3:D1:484:MET:HA	2.19	0.42
2:C1:175:THR:HG23	2:C1:175:THR:O	2.18	0.42
3:D8:38:ASP:OD2	3:D8:38:ASP:C	2.62	0.42
3:D4:173:TYR:O	3:D4:176:VAL:HG12	2.19	0.42
1:B2:83:ASN:CG	1:B2:84:GLU:N	2.77	0.42
1:B3:234:THR:HG23	1:B3:235:PRO:HD2	2.01	0.42
1:B6:285:THR:OG1	1:B6:286:PRO:HD2	2.19	0.42
3:DB:339:VAL:HG12	3:DB:340:LEU:N	2.32	0.42
4:P3:332:VAL:O	4:P3:370:LYS:HE2	2.19	0.42
1:B5:145:ALA:HB1	1:B5:146:PRO:HD2	2.01	0.42
1:B5:229:LEU:HB3	1:B5:230:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C6:320:THR:HG23	2:C6:321:PRO:HD3	2.00	0.42
3:D2:144:ALA:O	3:D2:147:VAL:HG12	2.19	0.42
1:B4:338:VAL:CG1	1:B4:339:ASN:N	2.82	0.42
3:D3:480:TYR:CD1	3:D3:480:TYR:N	2.86	0.42
1:B3:59:SER:OG	3:D3:484:MET:HA	2.20	0.42
1:B4:59:SER:OG	3:D9:484:MET:HA	2.18	0.42
2:C1:338:ILE:HD11	2:C1:357:TRP:CZ3	2.54	0.42
3:D6:24:GLY:O	3:D6:100:ARG:HA	2.20	0.42
1:B2:497:MET:O	1:B2:498:THR:HG22	2.20	0.42
2:C2:294:ALA:HA	2:C2:298:ALA:HB3	2.01	0.42
3:DC:135:ASP:HB2	3:DC:136:PRO:HD2	2.01	0.42
1:B5:267:GLY:N	1:B5:279:ILE:HG23	2.35	0.42
3:D1:347:ARG:CZ	3:D1:347:ARG:HB3	2.50	0.42
3:DB:42:PRO:O	3:DB:45:VAL:HG22	2.20	0.42
1:B2:90:ASP:C	1:B2:90:ASP:OD1	2.62	0.41
1:B4:90:ASP:OD1	1:B4:90:ASP:C	2.63	0.41
2:C1:338:ILE:HD11	2:C1:357:TRP:CH2	2.55	0.41
2:C4:175:THR:O	2:C4:175:THR:HG23	2.19	0.41
4:P3:148:MET:HE2	4:P3:471:ILE:HD11	2.02	0.41
3:D3:410:ARG:O	3:D3:412:GLN:N	2.52	0.41
3:D5:25:VAL:N	3:D5:33:ILE:O	2.51	0.41
3:D6:135:ASP:HB2	3:D6:136:PRO:HD2	2.01	0.41
4:P3:115:HIS:ND1	4:P3:116:PRO:HD2	2.35	0.41
1:B5:90:ASP:OD1	1:B5:90:ASP:C	2.63	0.41
3:D8:412:GLN:O	3:D8:415:THR:HG22	2.20	0.41
3:D9:195:ASP:N	3:D9:195:ASP:OD2	2.53	0.41
3:DA:144:ALA:O	3:DA:147:VAL:HG12	2.20	0.41
1:B6:40:TRP:CD1	1:B6:40:TRP:N	2.88	0.41
3:D7:25:VAL:HG13	3:D7:25:VAL:O	2.20	0.41
3:D9:275:ALA:O	3:D9:276:THR:HG22	2.20	0.41
4:P1:339:ASN:O	4:P1:339:ASN:CG	2.64	0.41
4:P3:42:PRO:HA	4:P3:43:PRO:HD3	1.97	0.41
1:B1:90:ASP:OD1	1:B1:90:ASP:C	2.63	0.41
1:B1:335:MET:HA	1:B1:336:PRO:HD3	1.95	0.41
1:B2:365:TRP:HD1	1:B2:366:TRP:N	2.19	0.41
2:C6:234:MET:HE1	2:C6:349:PHE:CG	2.55	0.41
3:DB:171:THR:HG23	3:DB:172:ILE:N	2.36	0.41
4:P2:413:ASP:OD2	4:P2:413:ASP:C	2.63	0.41
1:B2:213:ARG:NH1	1:B2:214:GLU:OE2	2.54	0.41
1:B3:90:ASP:OD1	1:B3:90:ASP:C	2.63	0.41
1:B6:90:ASP:OD1	1:B6:92:ASP:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D1:311:PHE:CD2	3:D1:312:PRO:HD2	2.56	0.41
3:D5:399:PHE:CD1	3:D5:399:PHE:C	2.99	0.41
3:D7:171:THR:HG23	3:D7:172:ILE:N	2.36	0.41
1:B1:385:ILE:CG2	1:B1:386:PRO:HD2	2.50	0.41
1:B4:304:THR:CG2	1:B4:305:LEU:N	2.83	0.41
2:C2:175:THR:HG23	2:C2:175:THR:O	2.21	0.41
2:C2:320:THR:HG23	2:C2:321:PRO:CD	2.50	0.41
3:D1:36:LEU:C	3:D1:36:LEU:HD23	2.46	0.41
3:D1:40:ASN:HA	3:D1:89:SER:HB3	2.02	0.41
3:D9:276:THR:HG23	3:D9:277:SER:N	2.36	0.41
3:D9:480:TYR:CD1	3:D9:480:TYR:N	2.87	0.41
3:DB:399:PHE:CD1	3:DB:399:PHE:C	2.98	0.41
3:D9:325:ASP:OD1	3:D9:325:ASP:N	2.53	0.41
3:DA:286:LEU:O	3:DA:290:VAL:HG23	2.21	0.41
4:P2:109:ASP:OD2	4:P2:110:THR:N	2.54	0.41
1:B4:356:ILE:H	1:B4:356:ILE:HD12	1.85	0.40
2:C1:346:VAL:HG12	2:C1:347:THR:N	2.36	0.40
2:C3:248:ASP:OD2	2:C3:248:ASP:N	2.54	0.40
2:C5:175:THR:HG23	2:C5:175:THR:O	2.21	0.40
2:C6:126:ASP:O	2:C6:130:ARG:HG2	2.21	0.40
3:DC:168:TRP:O	3:DC:171:THR:HG22	2.21	0.40
1:B2:92:ASP:OD2	1:B2:92:ASP:C	2.64	0.40
2:C3:151:ARG:HD3	2:C3:157:ASP:OD1	2.22	0.40
2:C5:38:TRP:CD1	2:C5:39:LEU:N	2.90	0.40
2:C6:320:THR:HG23	2:C6:321:PRO:CD	2.52	0.40
3:D9:484:MET:HB3	3:D9:485:PRO:HD3	2.02	0.40
4:P1:55:PRO:HA	4:P1:56:PRO:HD3	1.97	0.40
1:B2:46:ILE:HD11	1:B4:19:THR:HG22	2.02	0.40
1:B2:399:VAL:HB	1:B5:491:ASP:CG	2.47	0.40
1:B4:44:MET:O	1:B4:44:MET:HG3	2.20	0.40
1:B4:268:GLY:N	1:B4:279:ILE:HG22	2.36	0.40
2:C5:336:TYR:CZ	2:C5:337:VAL:HG23	2.57	0.40
1:B4:421:VAL:CG1	1:B4:467:ALA:HB3	2.51	0.40
1:B6:229:LEU:HB3	1:B6:230:PRO:HD3	2.03	0.40
2:C4:85:PHE:CG	2:C4:85:PHE:O	2.74	0.40
3:D3:25:VAL:O	3:D3:25:VAL:HG13	2.22	0.40
4:P1:413:ASP:OD2	4:P1:413:ASP:C	2.65	0.40
4:P3:409:VAL:HA	4:P3:431:ILE:O	2.21	0.40

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	B1	470/506 (93%)	457 (97%)	13 (3%)	0	100	100
1	B2	470/506 (93%)	464 (99%)	6 (1%)	0	100	100
1	B3	470/506 (93%)	456 (97%)	14 (3%)	0	100	100
1	B4	476/506 (94%)	469 (98%)	7 (2%)	0	100	100
1	B5	476/506 (94%)	468 (98%)	8 (2%)	0	100	100
1	B6	476/506 (94%)	467 (98%)	9 (2%)	0	100	100
2	C1	402/1391 (29%)	390 (97%)	11 (3%)	1 (0%)	43	75
2	C2	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	43	75
2	C3	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	43	75
2	C4	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	43	75
2	C5	402/1391 (29%)	391 (97%)	10 (2%)	1 (0%)	43	75
2	C6	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	43	75
3	D1	483/503 (96%)	477 (99%)	6 (1%)	0	100	100
3	D2	401/503 (80%)	395 (98%)	6 (2%)	0	100	100
3	D3	483/503 (96%)	471 (98%)	12 (2%)	0	100	100
3	D4	411/503 (82%)	403 (98%)	8 (2%)	0	100	100
3	D5	483/503 (96%)	475 (98%)	8 (2%)	0	100	100
3	D6	401/503 (80%)	392 (98%)	9 (2%)	0	100	100
3	D7	483/503 (96%)	472 (98%)	11 (2%)	0	100	100
3	D8	401/503 (80%)	393 (98%)	8 (2%)	0	100	100
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%)	474 (98%)	9 (2%)	0	100	100
3	DC	401/503 (80%)	392 (98%)	9 (2%)	0	100	100
4	P1	440/585 (75%)	422 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P2	440/585 (75%)	425 (97%)	15 (3%)	0	100	100
4	P3	440/585 (75%)	423 (96%)	17 (4%)	0	100	100
All	All	11884/19173 (62%)	11613 (98%)	265 (2%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C2	155	GLY
2	C1	155	GLY
2	C3	155	GLY
2	C4	155	GLY
2	C5	155	GLY
2	C6	155	GLY

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	B1	390/411 (95%)	390 (100%)	0	100	100
1	B2	390/411 (95%)	390 (100%)	0	100	100
1	B3	390/411 (95%)	389 (100%)	1 (0%)	86	85
1	B4	389/411 (95%)	388 (100%)	1 (0%)	86	85
1	B5	389/411 (95%)	386 (99%)	3 (1%)	73	77
1	B6	389/411 (95%)	388 (100%)	1 (0%)	86	85
2	C1	342/1137 (30%)	342 (100%)	0	100	100
2	C2	342/1137 (30%)	341 (100%)	1 (0%)	86	85
2	C3	342/1137 (30%)	341 (100%)	1 (0%)	86	85
2	C4	342/1137 (30%)	340 (99%)	2 (1%)	78	80
2	C5	342/1137 (30%)	341 (100%)	1 (0%)	86	85
2	C6	342/1137 (30%)	342 (100%)	0	100	100
3	D1	381/393 (97%)	379 (100%)	2 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D2	311/393 (79%)	310 (100%)	1 (0%)	86	85
3	D3	381/393 (97%)	379 (100%)	2 (0%)	81	82
3	D4	319/393 (81%)	318 (100%)	1 (0%)	86	85
3	D5	381/393 (97%)	379 (100%)	2 (0%)	81	82
3	D6	311/393 (79%)	310 (100%)	1 (0%)	86	85
3	D7	381/393 (97%)	380 (100%)	1 (0%)	86	85
3	D8	311/393 (79%)	311 (100%)	0	100	100
3	D9	381/393 (97%)	379 (100%)	2 (0%)	81	82
3	DA	311/393 (79%)	309 (99%)	2 (1%)	78	80
3	DB	381/393 (97%)	380 (100%)	1 (0%)	86	85
3	DC	311/393 (79%)	310 (100%)	1 (0%)	86	85
4	P1	343/453 (76%)	343 (100%)	0	100	100
4	P2	343/453 (76%)	343 (100%)	0	100	100
4	P3	343/453 (76%)	343 (100%)	0	100	100
All	All	9578/15363 (62%)	9551 (100%)	27 (0%)	84	85

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B3	29	LEU
1	B4	73	TRP
1	B5	125	LEU
1	B5	285	THR
1	B5	332	LEU
1	B6	285	THR
2	C2	58	PHE
2	C3	151	ARG
2	C4	37	TRP
2	C4	58	PHE
2	C5	38	TRP
3	D1	399	PHE
3	D1	431	TYR
3	D2	117	GLU
3	D3	399	PHE
3	D3	435	LEU
3	D4	130	ARG
3	D5	399	PHE

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Mol	Chain	Res	Type
3	D5	431	TYR
3	D6	117	GLU
3	D7	399	PHE
3	D9	399	PHE
3	D9	431	TYR
3	DA	117	GLU
3	DA	130	ARG
3	DB	399	PHE
3	DC	163	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	B1	287	GLN
1	B1	359	HIS
1	B1	417	HIS
1	B2	315	ASN
1	B2	339	ASN
1	B3	81	GLN
1	B3	315	ASN
1	B4	83	ASN
1	B4	477	GLN
1	B5	22	GLN
1	B6	130	GLN
2	C2	159	ASN
2	C2	261	GLN
2	C3	93	GLN
2	C3	261	GLN
2	C4	261	GLN
2	C5	245	HIS
2	C5	261	GLN
2	C6	92	GLN
2	C6	133	HIS
2	C6	159	ASN
2	C6	261	GLN
2	C6	322	HIS
3	D1	165	HIS
3	D1	461	HIS
3	D1	495	ASN
3	D2	114	GLN
3	D2	164	HIS
3	D2	412	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D3	165	HIS
3	D3	495	ASN
3	D4	118	HIS
3	D5	461	HIS
3	D5	495	ASN
3	D6	412	GLN
3	D7	32	GLN
3	D8	412	GLN
3	D9	461	HIS
3	DB	32	GLN
3	DB	495	ASN
3	DC	114	GLN
4	P1	82	GLN
4	P1	391	ASN
4	P1	450	ASN
4	P2	283	GLN
4	P2	328	ASN
4	P2	391	ASN
4	P2	450	ASN
4	P2	497	HIS
4	P3	82	GLN
4	P3	391	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](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

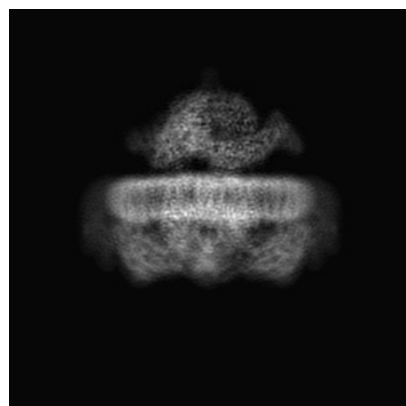
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12514. These allow visual inspection of the internal detail of the map and identification of artifacts.

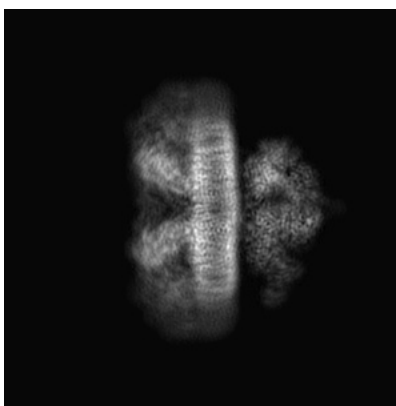
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

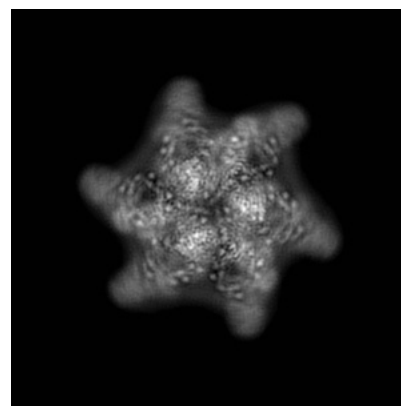
6.1.1 Primary map



X

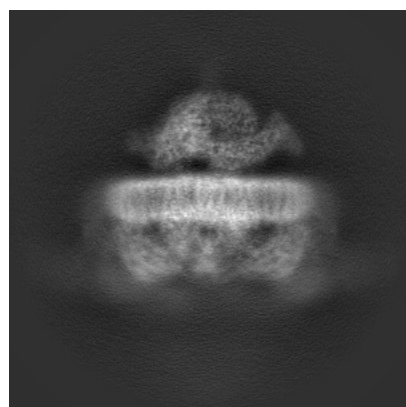


Y

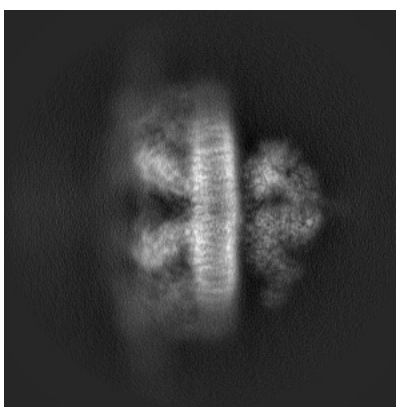


Z

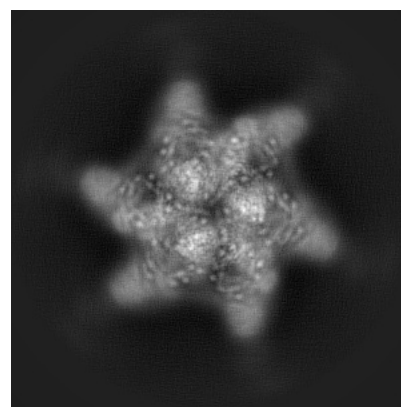
6.1.2 Raw map



X



Y

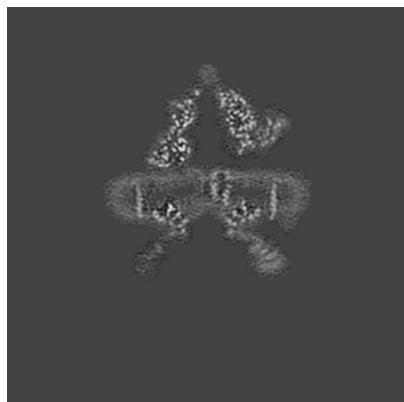


Z

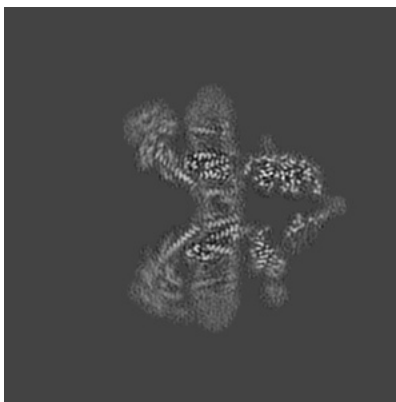
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

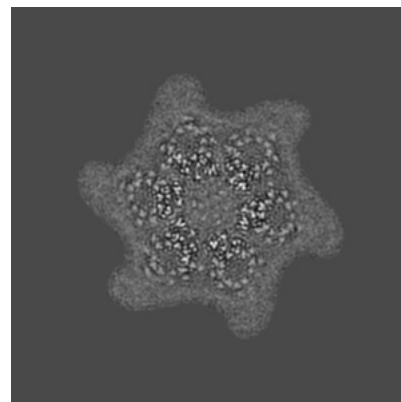
6.2.1 Primary map



X Index: 200

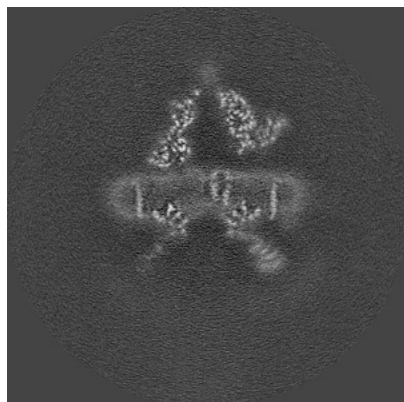


Y Index: 200

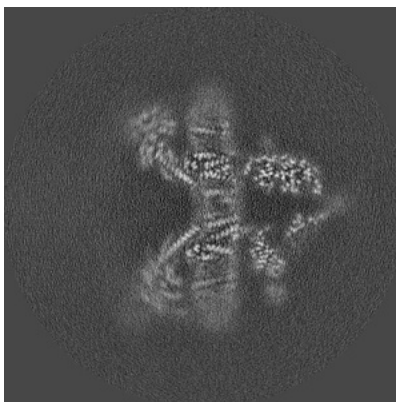


Z Index: 200

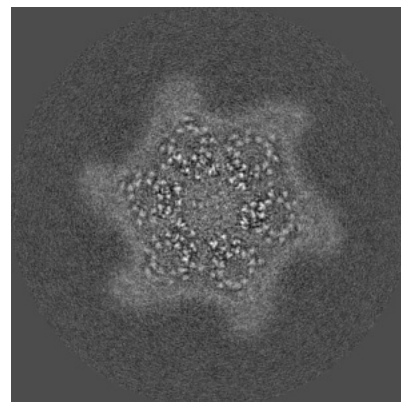
6.2.2 Raw map



X Index: 200



Y Index: 200

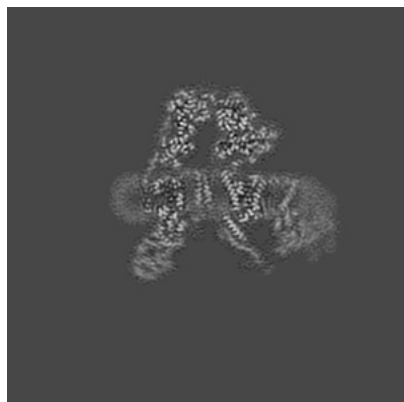


Z Index: 200

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

6.3 Largest variance slices [i](#)

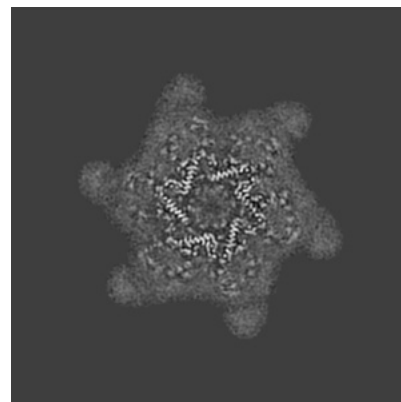
6.3.1 Primary map



X Index: 184

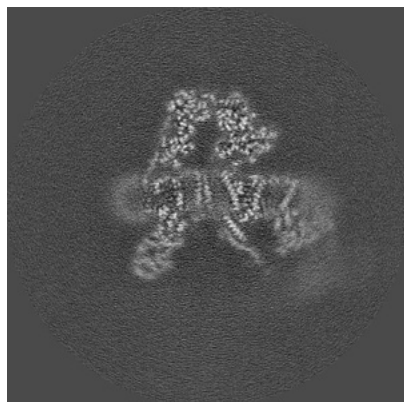


Y Index: 199

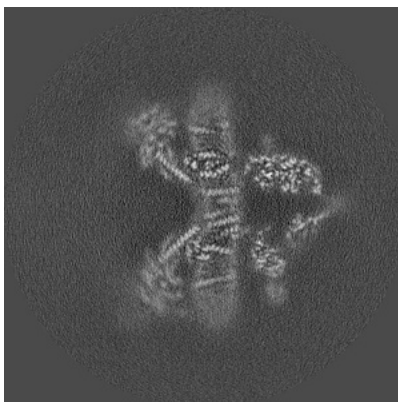


Z Index: 192

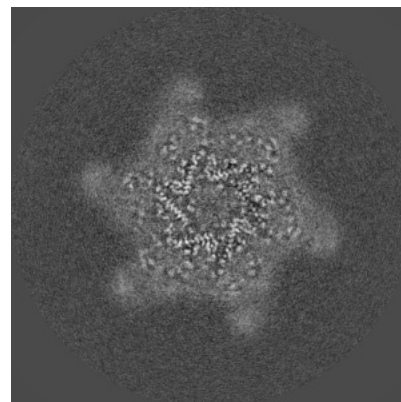
6.3.2 Raw map



X Index: 184



Y Index: 199

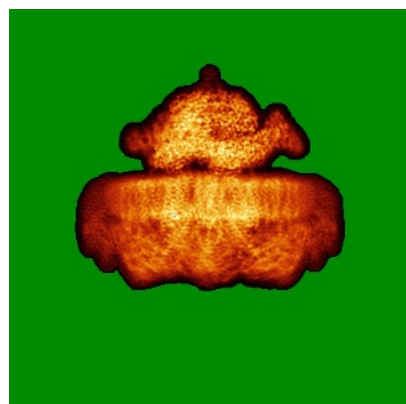


Z Index: 193

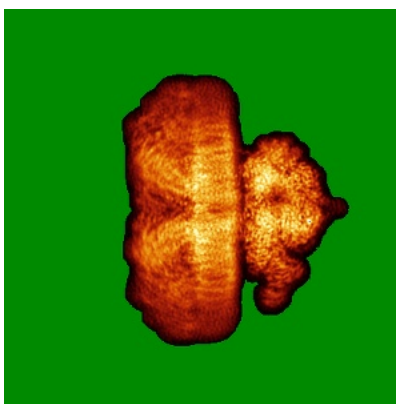
The images above show the largest variance slices of the map in three orthogonal directions.

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

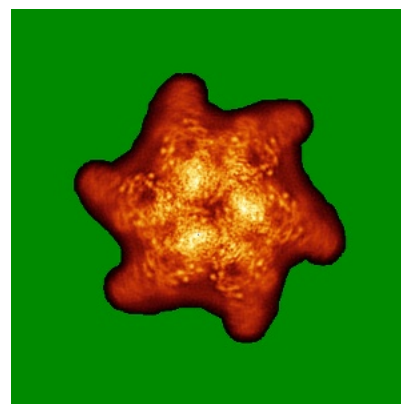
6.4.1 Primary map



X

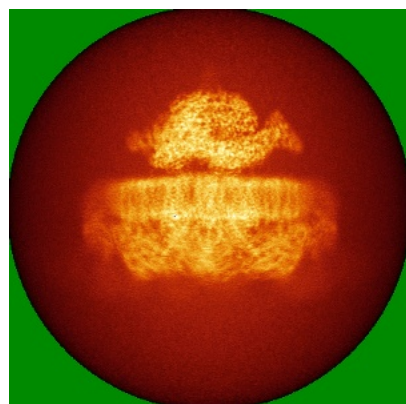


Y

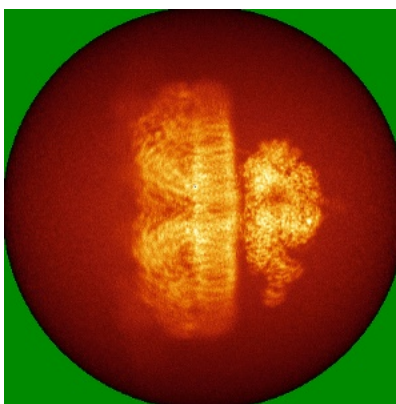


Z

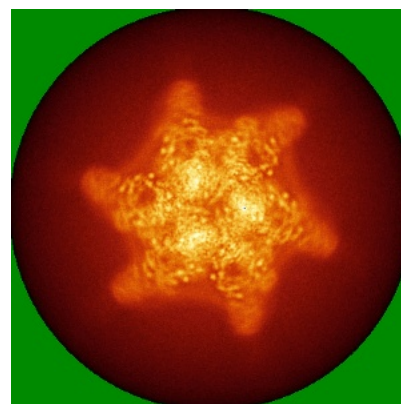
6.4.2 Raw map



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](#)

This section was not generated.

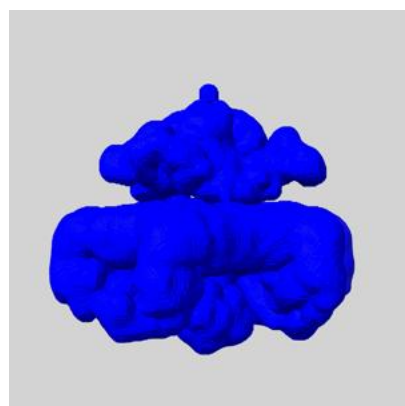
6.6 Mask visualisation [i](#)

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

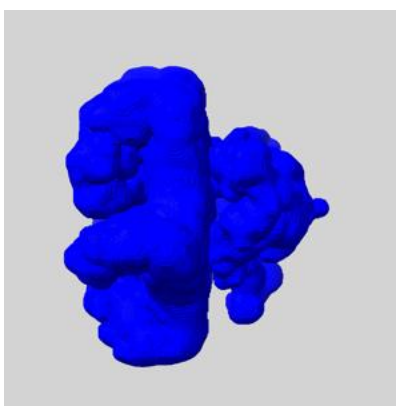
A mask typically either:

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

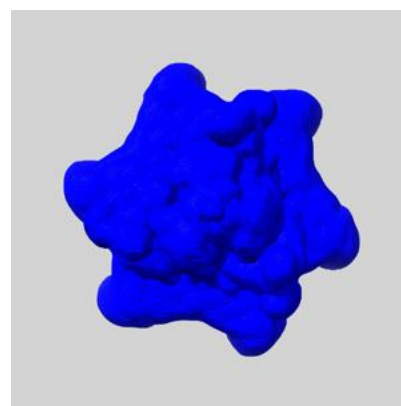
6.6.1 emd_12514_msk_1.map [i](#)



X



Y

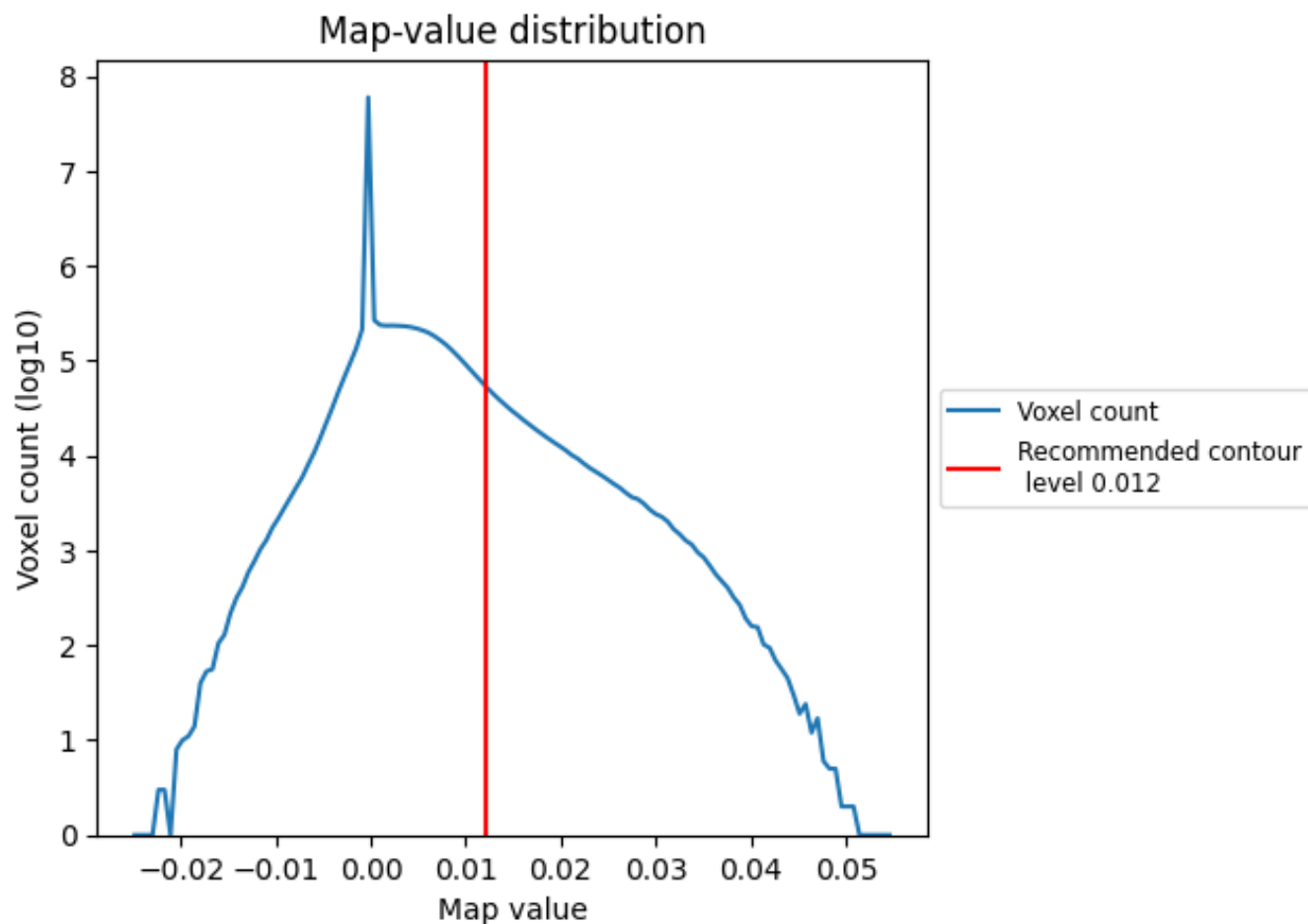


Z

7 Map analysis [i](#)

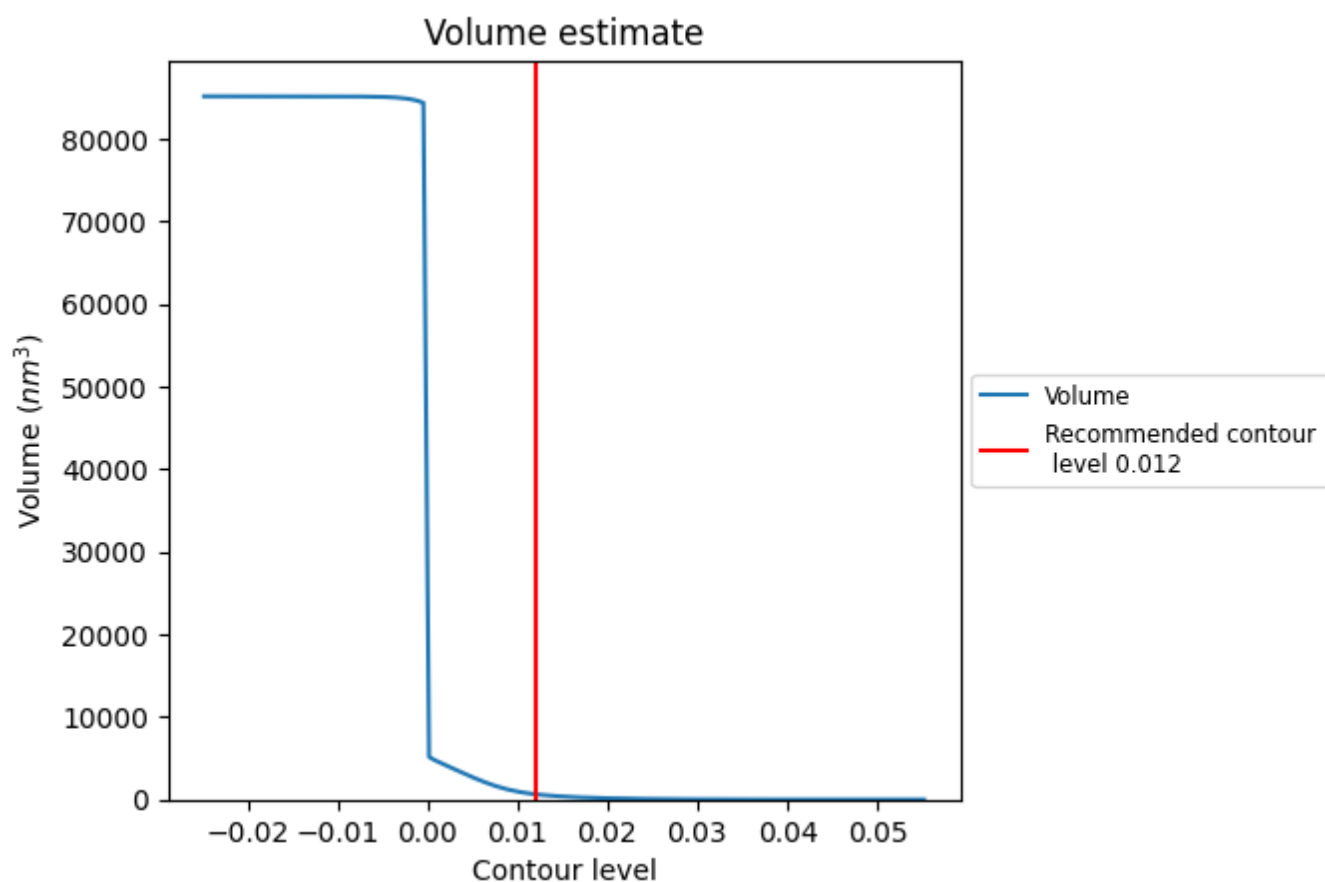
This section contains the results of statistical analysis of the map.

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.

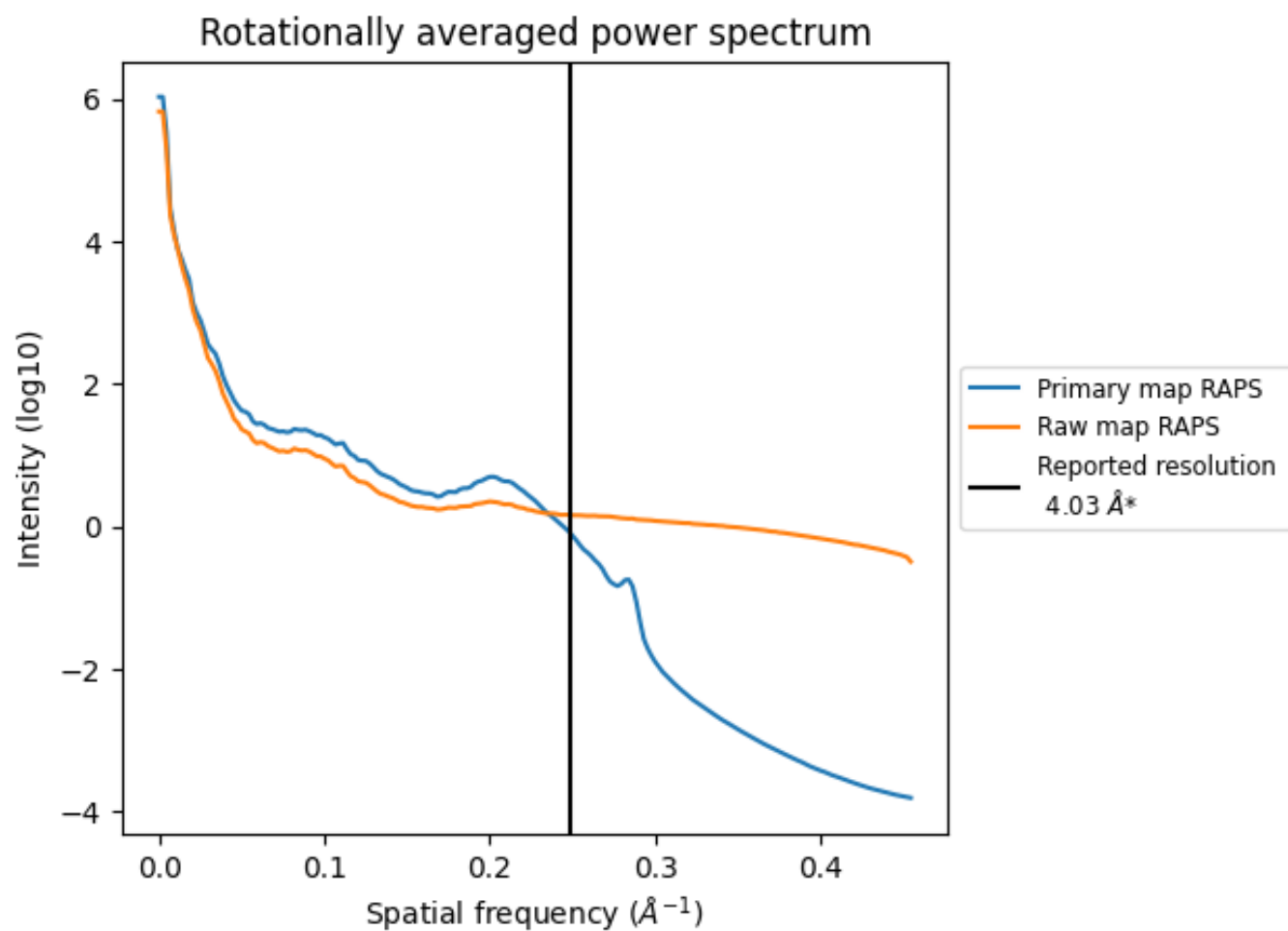
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 643 nm³; this corresponds to an approximate mass of 581 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 ⓘ

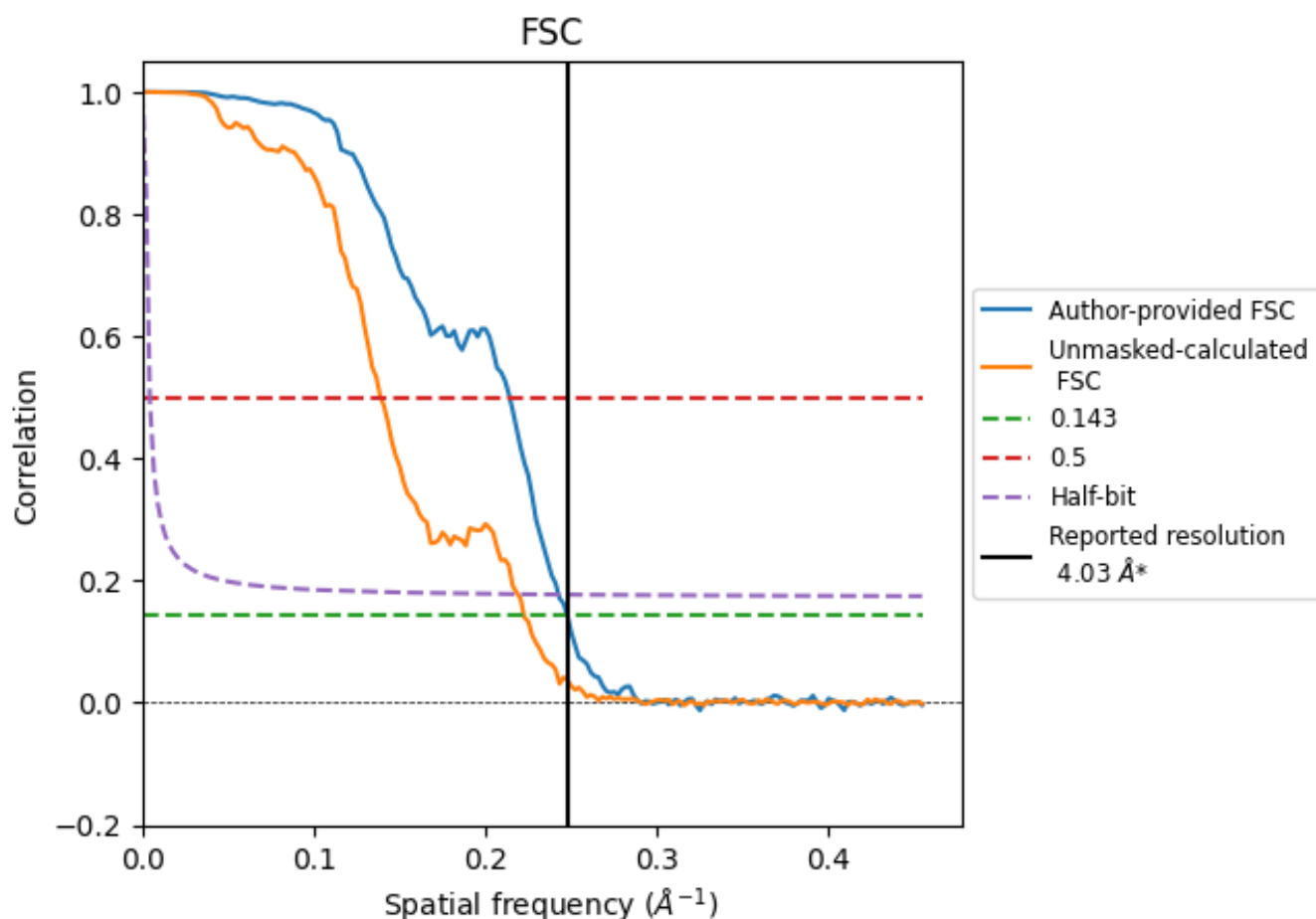


*Reported resolution corresponds to spatial frequency of 0.248 $\text{\AA}^{-1}$

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 $0.248 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.03	-	-
Author-provided FSC curve	4.04	4.67	4.12
Unmasked-calculated*	4.49	7.19	4.57

*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 4.49 differs from the reported value 4.03 by more than 10 %

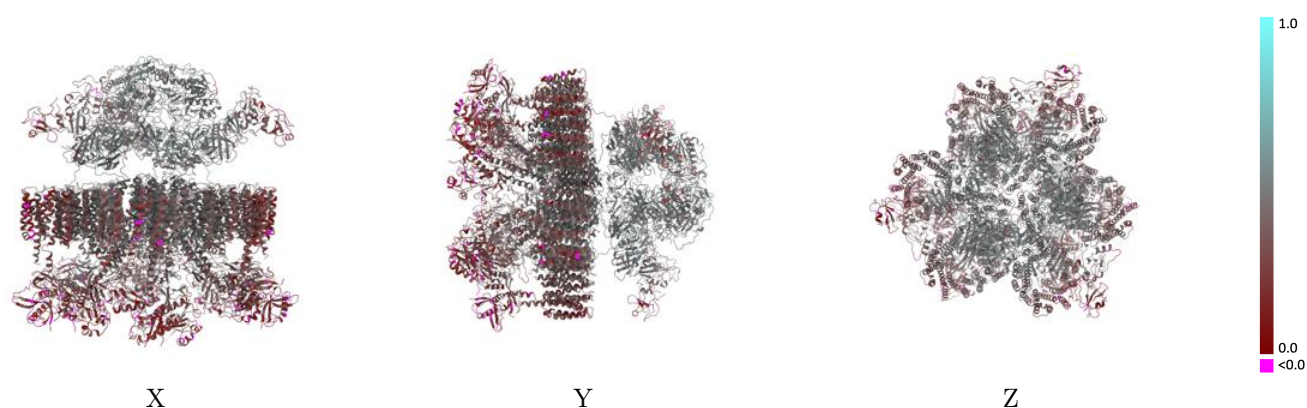
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12514 and PDB model 7NP7. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

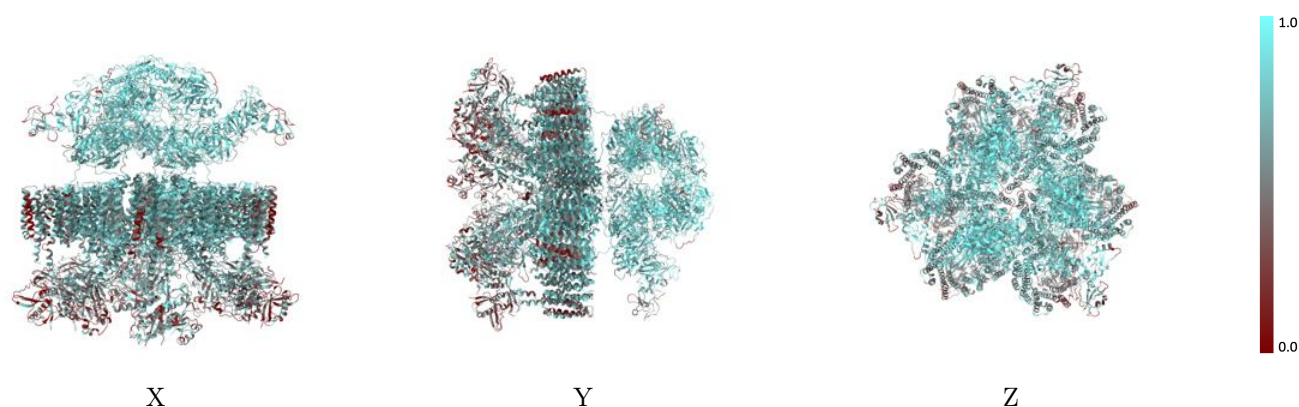
This section was not generated.

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



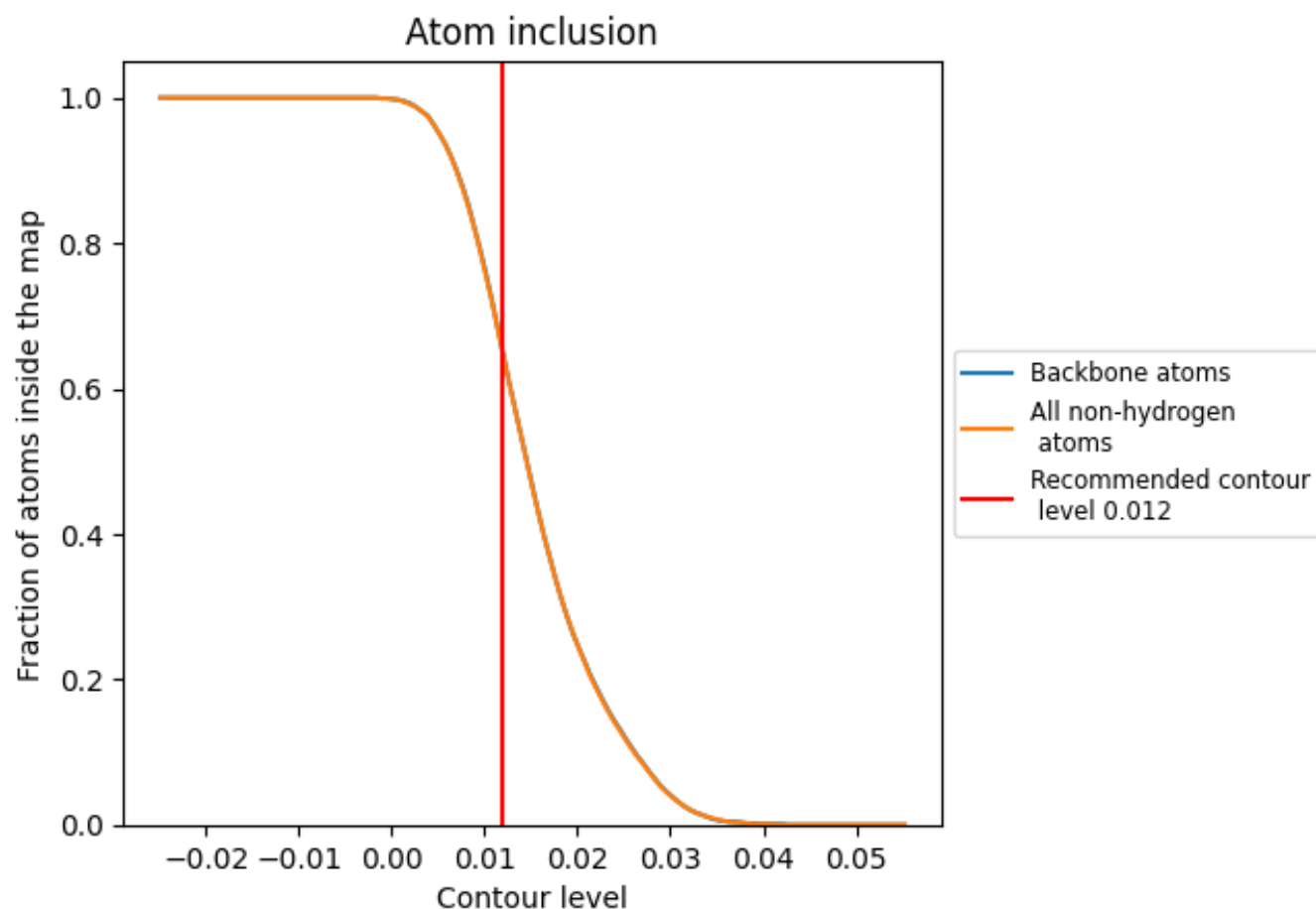
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.3830
B1	 0.7560	 0.4350
B2	 0.7520	 0.4340
B3	 0.7460	 0.4370
B4	 0.8020	 0.4640
B5	 0.7990	 0.4670
B6	 0.8040	 0.4690
C1	 0.5940	 0.3420
C2	 0.5030	 0.3010
C3	 0.5960	 0.3340
C4	 0.4950	 0.2960
C5	 0.5970	 0.3310
C6	 0.4970	 0.3000
D1	 0.6130	 0.3480
D2	 0.5510	 0.3160
D3	 0.6820	 0.4000
D4	 0.5990	 0.3450
D5	 0.6090	 0.3480
D6	 0.5460	 0.3110
D7	 0.6820	 0.3960
D8	 0.5990	 0.3530
D9	 0.6060	 0.3490
DA	 0.5550	 0.3150
DB	 0.6840	 0.4000
DC	 0.5990	 0.3430
P1	 0.8190	 0.4760
P2	 0.8130	 0.4760
P3	 0.8140	 0.4780

