Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 08:50 AM EST

PDB ID	:	6V0F
EMDB ID	:	EMD-20996
Title	:	Lipophilic Envelope-spanning Tunnel B (LetB), Model 4
Authors	:	Isom, G.L.; Coudray, N.; MacRae, M.R.; McManus, C.T.; Ekiert, D.C.; Bhabha, G.
Deposited on	:	2019-11-18
Resolution	:	2.96 Å(reported)
Based on initial model	:	5UW2

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:

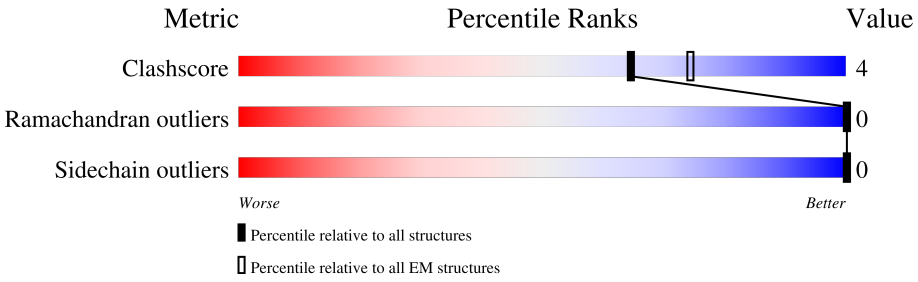
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.96 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 <=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	832	7% 36% 6% 58%
1	B	832	8% 36% 6% 58%
1	C	832	7% 37% 5% 58%
1	D	832	7% 37% 6% 58%
1	E	832	8% 37% 6% 58%
1	F	832	7% 36% 6% 58%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15942 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.

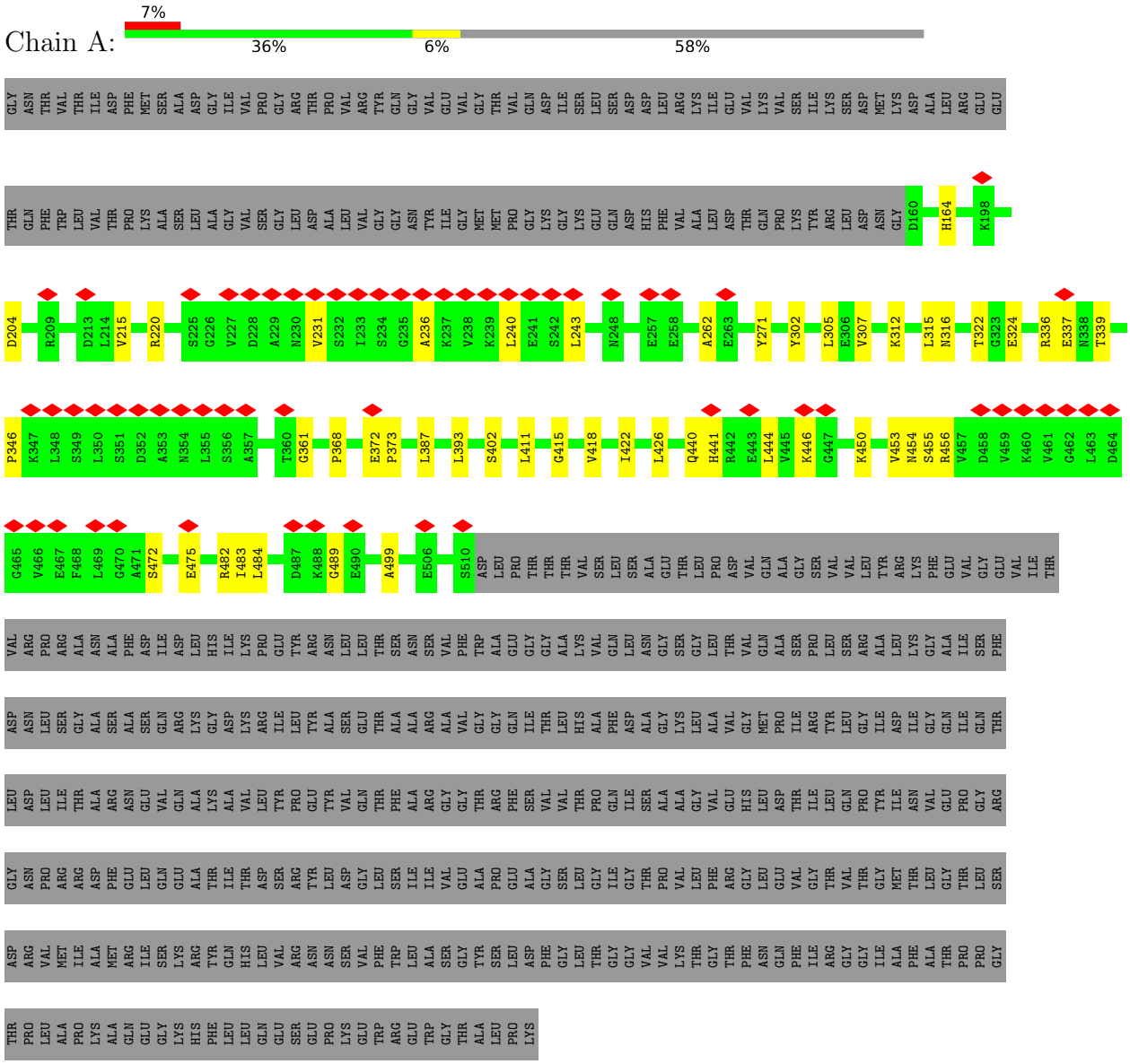
- Molecule 1 is a protein called Intermembrane transport protein YebT.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	B	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	C	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	D	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	E	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		
1	F	351	Total	C	N	O	S	0	0
			2657	1688	448	517	4		

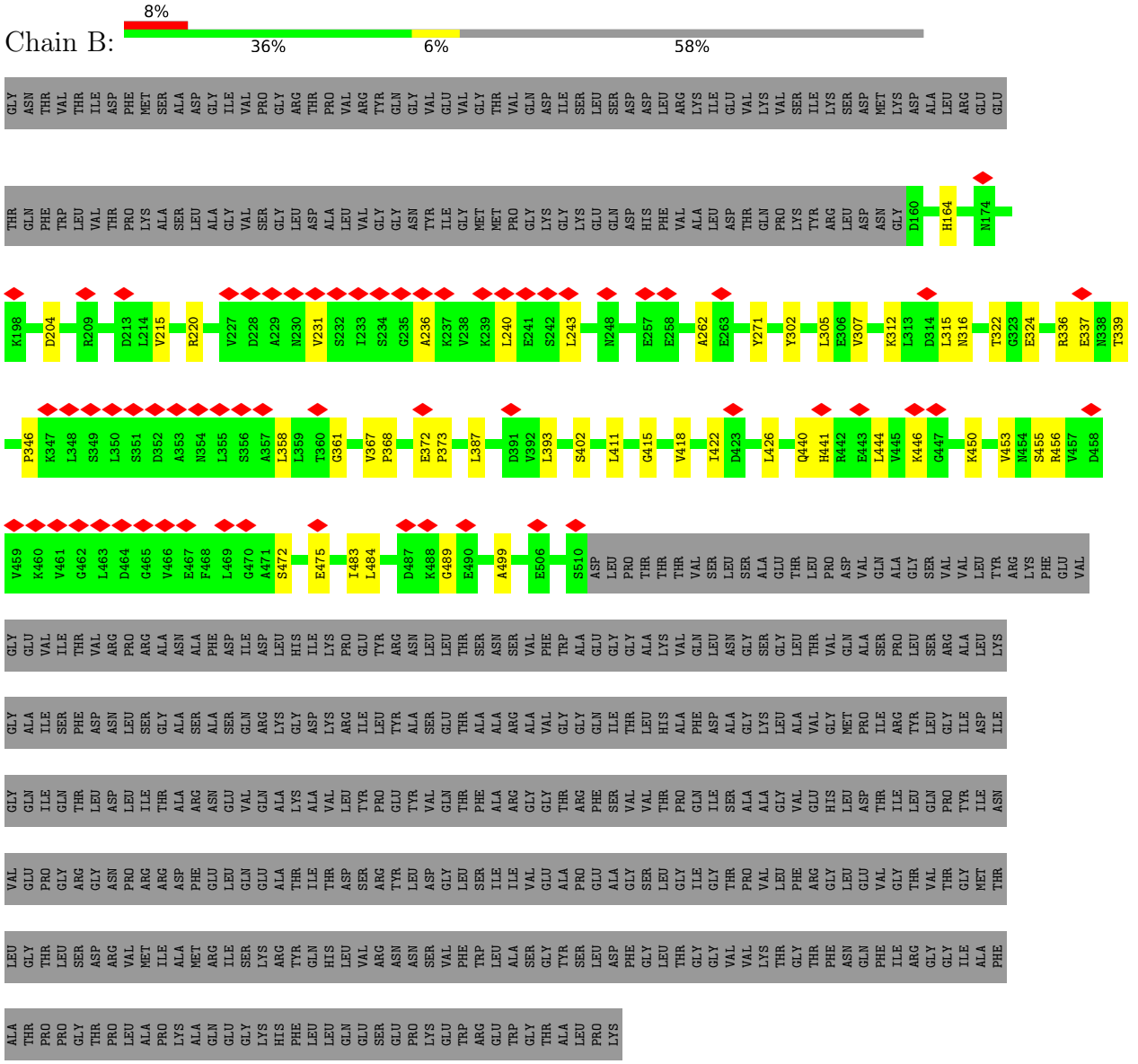
3 Residue-property plots (i)

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.

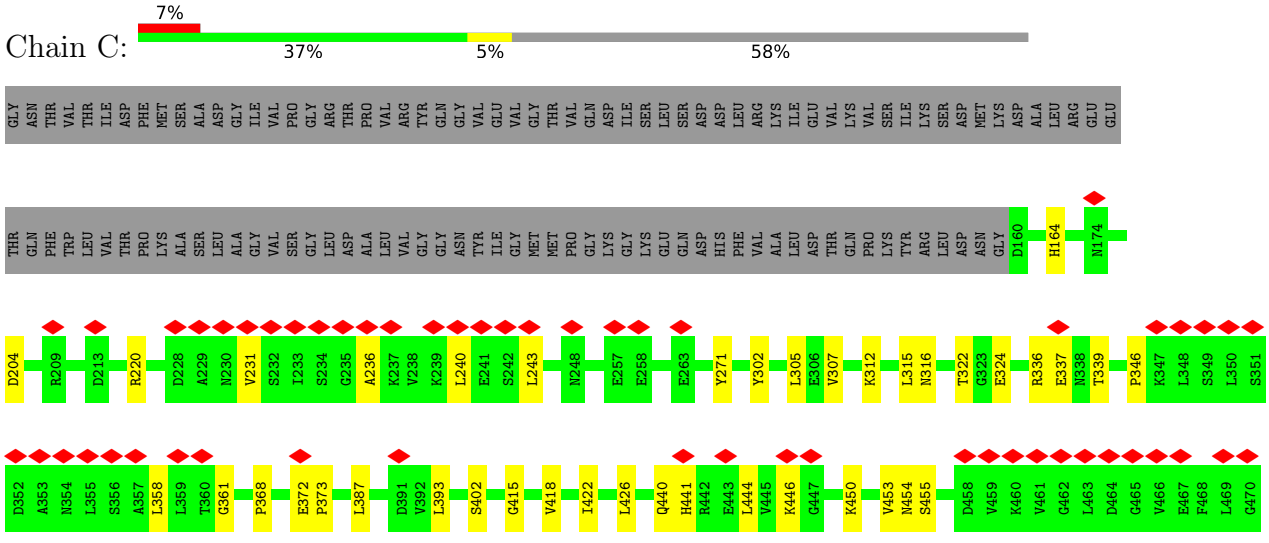
• Molecule 1: Intermembrane transport protein YebT

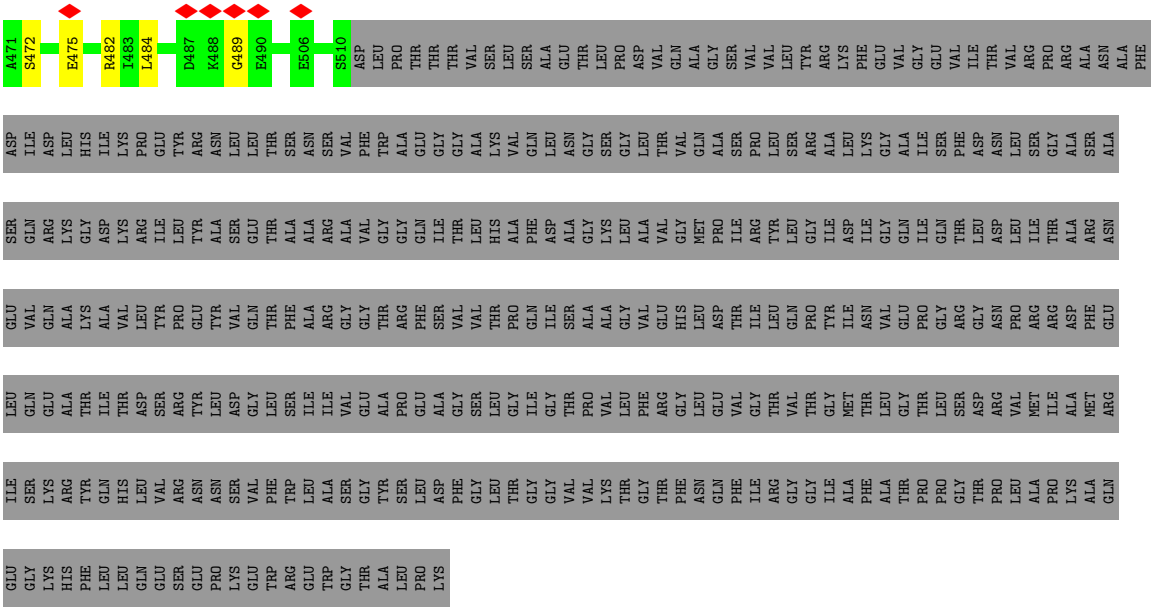


• Molecule 1: Intermembrane transport protein YebT

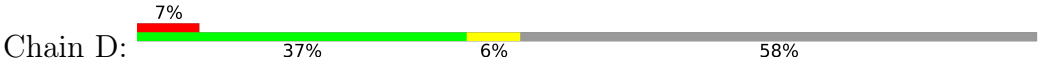


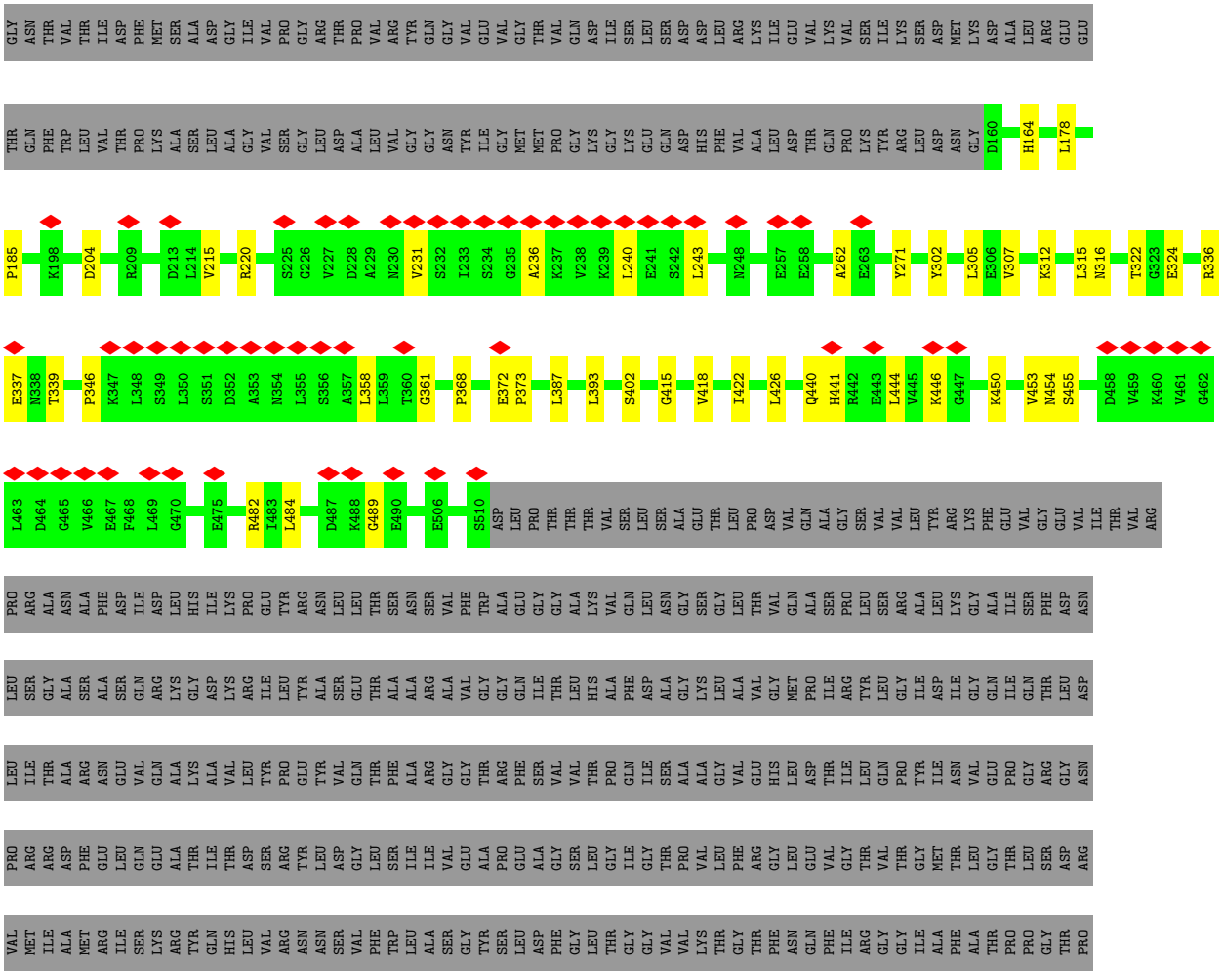
• Molecule 1: Intermembrane transport protein YebT



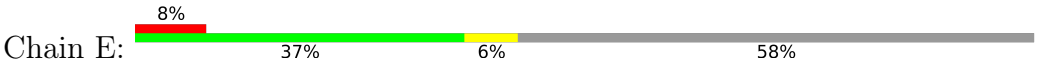


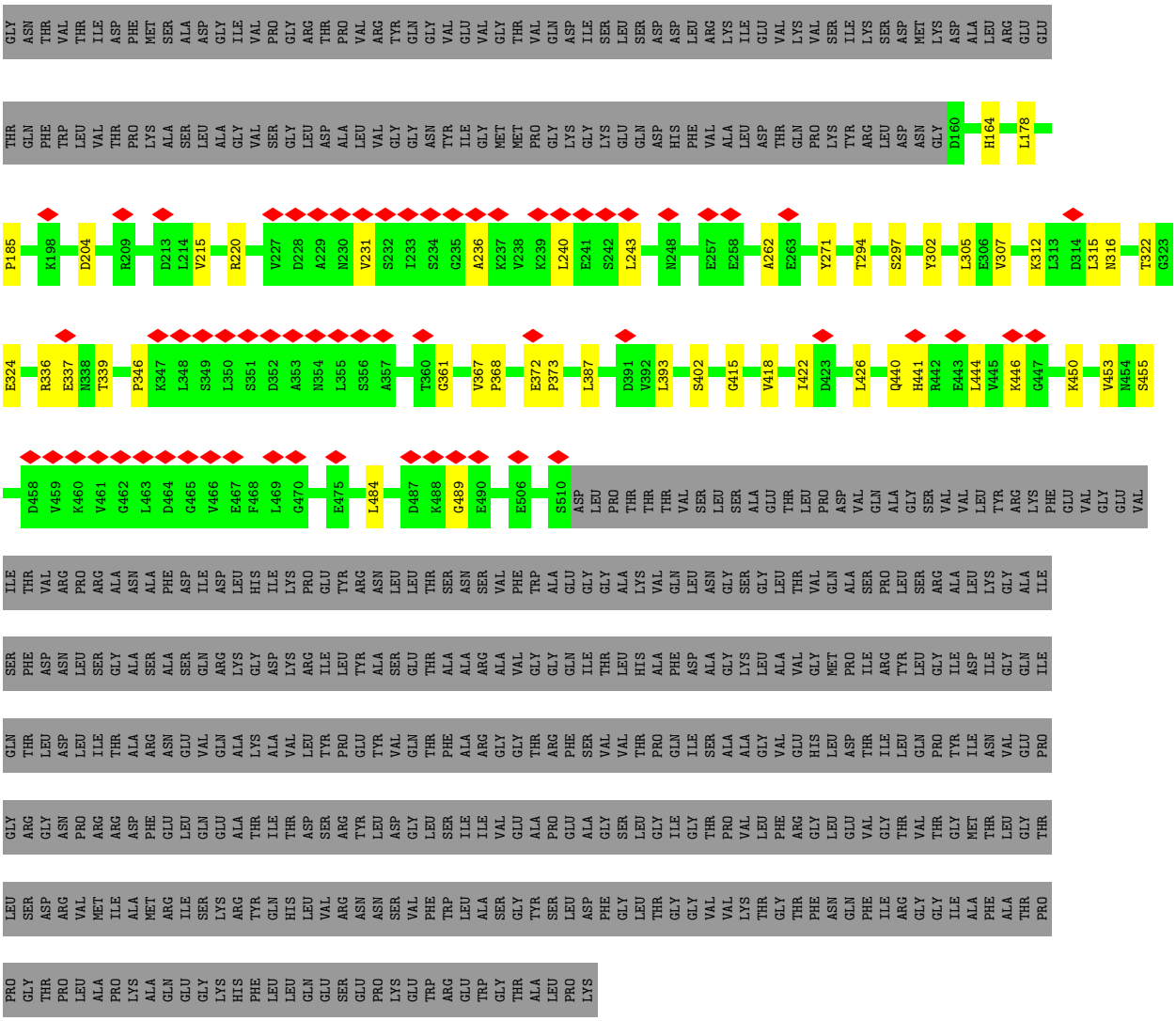
- Molecule 1: Intermembrane transport protein YebT



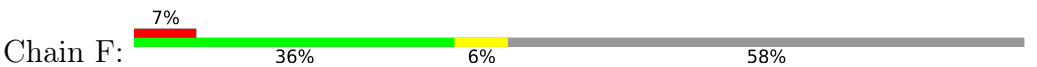


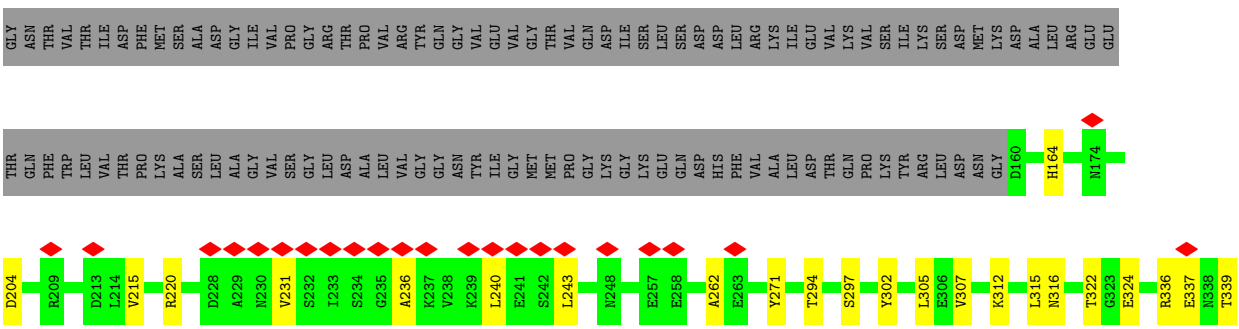
• Molecule 1: Intermembrane transport protein YebT

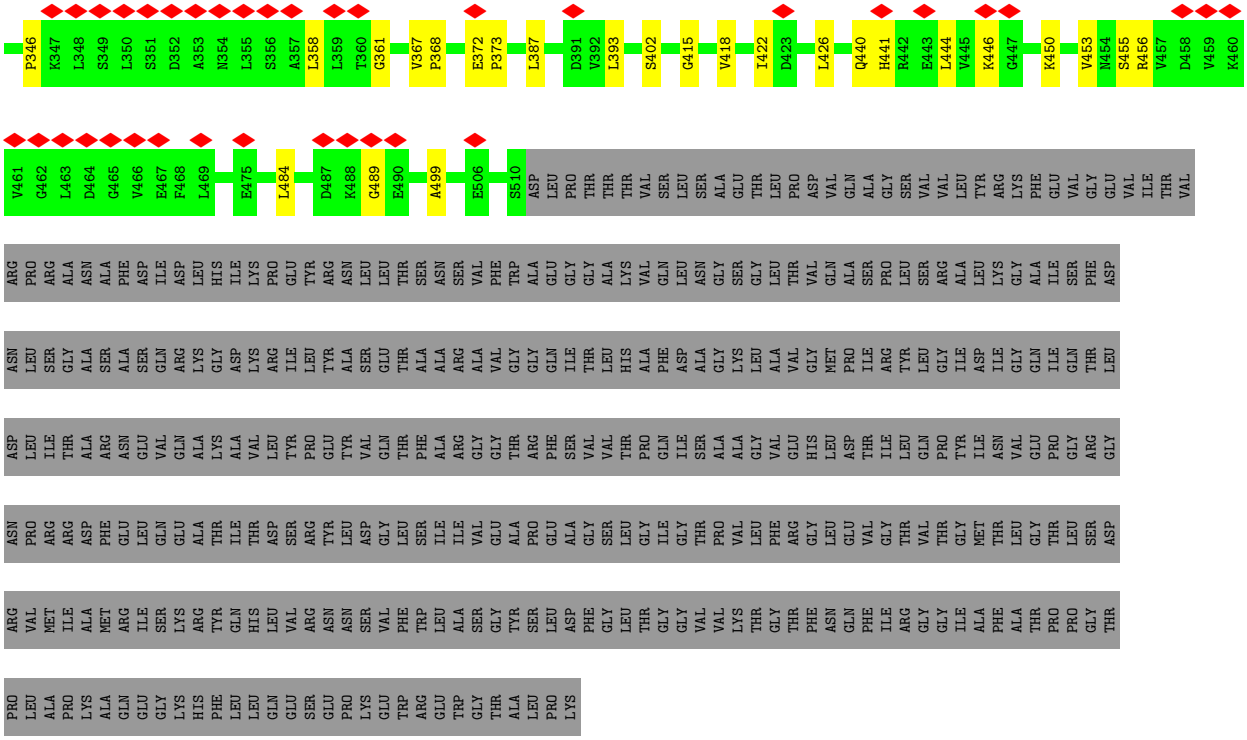




• Molecule 1: Intermembrane transport protein YebT






P346 K347 L348 S349 L350 S351 D352 A353 N354 L355 S356 A357 L358 L359 T360 G361 V367 P368 E372 P373 L387 D391 V392 L393 S402 G415 V418 I422 D423 L426 Q440 H441 R442 E443 L444 V445 K446 G447 K450 V453 N454 S455 R456 V457 D458 V459 K460
V461 G462 L463 D464 G465 V466 E467 F468 L469 E475 L484 D487 K488 G489 E490 A499 E506 S510 ASP LEU PRO THR THR THR VAL SER LEU SER ALA GLU THR LEU PRO ASP VAL GLN ALA GLY SER VAL VAL LEU TYR ARG LYS PHE GLU VAL GLY GLU VAL ILE THR VAL
ARG PRO ARG ALA ASN ALA PHE ASP ILE ASP LEU HIS ILE LYS PRO GLU TYR ARG ASN LEU LEU THR SER ASN SER VAL PHE TRP ALA GLU GLY GLY ALA LYS VAL GLN LEU ASN GLY SER GLY LEU THR VAL PRO ASP VAL GLN ALA SER PRO LEU SER ARG ALA LEU LYS GLY ALA ILE SER PHE ASP
ASN LEU SER GLY ALA SER ALA SER GLN ARG LYS GLY ASP LYS ARG ILE LEU TYR ALA SER GLU THR ALA ALA ALA ARG ALA VAL GLY GLY GLN ILE THR LEU HIS ALA PHE ASP ALA GLY LYS LEU ALA VAL GLY MET PRO ILE ARG TYR LEU GLY ILE ASP ILE GLY GLN ILE GLN THR LEU
ASP LEU ILE THR ALA ARG ASN GLU VAL GLN ALA LYS ALA VAL LEU TYR PRO GLU TYR VAL GLN THR PHE ALA ARG GLY GLY THR ARG PHE SER VAL VAL THR PRO GLN ILE SER ALA ALA GLY VAL GLU HIS LEU ASP THR ILE LEU GLN PRO TYR ILE ASN VAL GLU PRO GLY ARG GLY
ASN PRO ARG ARG ASP PHE GLU LEU GLN GLU ALA THR ILE THR ASP SER ARG TYR LEU ASP GLY LEU SER ILE ILE VAL GLU ALA PRO GLU ALA GLY SER LEU GLY ILE GLY THR PRO VAL LEU PHE ARG GLY LEU GLU VAL GLY THR VAL THR GLY MET THR LEU GLY THR LEU SER ASP
ARG VAL MET ILE ALA MET ARG ILE SER LYS ARG TYR GLN HIS LEU VAL ARG ASN ASN SER VAL PHE TRP LEU ALA SER GLY TYR SER LEU ASP PHE GLY LEU THR GLY GLY VAL VAL LYS THR GLY THR PHE ASN GLN PHE ILE ARG GLY GLY ILE ALA PHE ALA THR PRO PRO GLY THR
PRO LEU ALA PRO LYS ALA GLN GLU GLY LYS HIS PHE LEU LEU GLN GLU SER GLU PRO LYS GLU TRP ARG GLU TRP GLY THR ALA LEU PRO LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	144219	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.529	Depositor
Minimum map value	-0.287	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	366.8, 366.8, 366.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	A	0.46	0/2702	0.74	4/3666 (0.1%)
1	B	0.46	0/2702	0.74	4/3666 (0.1%)
1	C	0.46	0/2702	0.74	4/3666 (0.1%)
1	D	0.46	0/2702	0.74	4/3666 (0.1%)
1	E	0.46	0/2702	0.74	4/3666 (0.1%)
1	F	0.46	0/2702	0.74	4/3666 (0.1%)
All	All	0.46	0/16212	0.74	24/21996 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	240	LEU	CA-CB-CG	9.09	136.21	115.30
1	C	240	LEU	CA-CB-CG	9.08	136.19	115.30
1	F	240	LEU	CA-CB-CG	9.08	136.19	115.30
1	D	240	LEU	CA-CB-CG	9.07	136.17	115.30
1	B	240	LEU	CA-CB-CG	9.07	136.17	115.30
1	A	240	LEU	CA-CB-CG	9.07	136.16	115.30
1	B	393	LEU	CA-CB-CG	6.49	130.22	115.30
1	F	393	LEU	CA-CB-CG	6.48	130.19	115.30
1	E	393	LEU	CA-CB-CG	6.47	130.17	115.30
1	C	393	LEU	CA-CB-CG	6.46	130.16	115.30
1	D	393	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	393	LEU	CA-CB-CG	6.45	130.13	115.30
1	F	426	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	243	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	426	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	426	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	243	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	243	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	426	LEU	CA-CB-CG	5.21	127.28	115.30
1	F	243	LEU	CA-CB-CG	5.21	127.29	115.30
1	E	243	LEU	CA-CB-CG	5.21	127.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	426	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	243	LEU	CA-CB-CG	5.20	127.27	115.30
1	E	426	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2657	0	2711	26	0
1	B	2657	0	2711	27	0
1	C	2657	0	2711	24	0
1	D	2657	0	2711	25	0
1	E	2657	0	2711	25	0
1	F	2657	0	2711	26	0
All	All	15942	0	16266	135	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 4.

All (135) 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:E:231:VAL:HB	1:F:236:ALA:H	1.63	0.63
1:E:336:ARG:HA	1:E:373:PRO:HA	1.82	0.62
1:A:336:ARG:HA	1:A:373:PRO:HA	1.82	0.62
1:B:336:ARG:HA	1:B:373:PRO:HA	1.82	0.62
1:D:231:VAL:HB	1:E:236:ALA:H	1.65	0.62
1:A:236:ALA:H	1:F:231:VAL:HB	1.65	0.61
1:A:231:VAL:HB	1:B:236:ALA:H	1.65	0.61
1:B:231:VAL:HB	1:C:236:ALA:H	1.64	0.61
1:D:336:ARG:HA	1:D:373:PRO:HA	1.82	0.61
1:F:336:ARG:HA	1:F:373:PRO:HA	1.82	0.61
1:D:450:LYS:HB2	1:D:484:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:450:LYS:HB2	1:F:484:LEU:HB2	1.83	0.61
1:C:336:ARG:HA	1:C:373:PRO:HA	1.81	0.60
1:A:450:LYS:HB2	1:A:484:LEU:HB2	1.83	0.60
1:C:450:LYS:HB2	1:C:484:LEU:HB2	1.83	0.60
1:C:231:VAL:HB	1:D:236:ALA:H	1.66	0.60
1:E:450:LYS:HB2	1:E:484:LEU:HB2	1.82	0.60
1:B:450:LYS:HB2	1:B:484:LEU:HB2	1.83	0.59
1:D:302:TYR:HB3	1:D:307:VAL:HG21	1.90	0.54
1:A:441:HIS:HA	1:A:444:LEU:HB2	1.90	0.54
1:E:302:TYR:HB3	1:E:307:VAL:HG21	1.90	0.54
1:B:441:HIS:HA	1:B:444:LEU:HB2	1.90	0.54
1:D:312:LYS:HB3	1:D:324:GLU:HG2	1.90	0.54
1:E:312:LYS:HB3	1:E:324:GLU:HG2	1.90	0.54
1:C:312:LYS:HB3	1:C:324:GLU:HG2	1.90	0.54
1:D:418:VAL:HA	1:D:440:GLN:HE21	1.73	0.54
1:C:302:TYR:HB3	1:C:307:VAL:HG21	1.90	0.54
1:C:418:VAL:HA	1:C:440:GLN:HE21	1.73	0.54
1:E:418:VAL:HA	1:E:440:GLN:HE21	1.73	0.54
1:F:418:VAL:HA	1:F:440:GLN:HE21	1.73	0.54
1:D:441:HIS:HA	1:D:444:LEU:HB2	1.89	0.53
1:E:453:VAL:HG12	1:E:455:SER:H	1.74	0.53
1:F:302:TYR:HB3	1:F:307:VAL:HG21	1.90	0.53
1:F:441:HIS:HA	1:F:444:LEU:HB2	1.90	0.53
1:F:312:LYS:HB3	1:F:324:GLU:HG2	1.90	0.53
1:F:453:VAL:HG12	1:F:455:SER:H	1.74	0.53
1:B:302:TYR:HB3	1:B:307:VAL:HG21	1.90	0.53
1:C:441:HIS:HA	1:C:444:LEU:HB2	1.89	0.53
1:B:312:LYS:HB3	1:B:324:GLU:HG2	1.90	0.53
1:B:453:VAL:HG12	1:B:455:SER:H	1.74	0.53
1:C:453:VAL:HG12	1:C:455:SER:H	1.74	0.53
1:A:302:TYR:HB3	1:A:307:VAL:HG21	1.90	0.53
1:A:418:VAL:HA	1:A:440:GLN:HE21	1.73	0.53
1:B:402:SER:HB3	1:C:415:GLY:HA3	1.91	0.53
1:E:441:HIS:HA	1:E:444:LEU:HB2	1.90	0.52
1:B:418:VAL:HA	1:B:440:GLN:HE21	1.73	0.52
1:D:453:VAL:HG12	1:D:455:SER:H	1.74	0.52
1:E:402:SER:HB3	1:F:415:GLY:HA3	1.92	0.52
1:A:312:LYS:HB3	1:A:324:GLU:HG2	1.90	0.52
1:A:415:GLY:HA3	1:F:402:SER:HB3	1.91	0.52
1:A:453:VAL:HG12	1:A:455:SER:H	1.74	0.52
1:C:220:ARG:NH2	1:C:271:TYR:OH	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:NH2	1:A:271:TYR:OH	2.43	0.52
1:F:220:ARG:NH2	1:F:271:TYR:OH	2.43	0.51
1:D:316:ASN:ND2	1:D:322:THR:OG1	2.44	0.51
1:D:402:SER:HB3	1:E:415:GLY:HA3	1.92	0.51
1:E:316:ASN:ND2	1:E:322:THR:OG1	2.44	0.51
1:B:220:ARG:NH2	1:B:271:TYR:OH	2.43	0.51
1:E:220:ARG:NH2	1:E:271:TYR:OH	2.43	0.51
1:D:220:ARG:NH2	1:D:271:TYR:OH	2.43	0.51
1:B:316:ASN:ND2	1:B:322:THR:OG1	2.44	0.51
1:C:316:ASN:ND2	1:C:322:THR:OG1	2.44	0.51
1:A:402:SER:HB3	1:B:415:GLY:HA3	1.92	0.51
1:F:316:ASN:ND2	1:F:322:THR:OG1	2.44	0.51
1:A:316:ASN:ND2	1:A:322:THR:OG1	2.44	0.50
1:C:402:SER:HB3	1:D:415:GLY:HA3	1.93	0.49
1:B:387:LEU:HD22	1:B:422:ILE:HG21	1.96	0.48
1:D:387:LEU:HD22	1:D:422:ILE:HG21	1.96	0.47
1:A:387:LEU:HD22	1:A:422:ILE:HG21	1.96	0.47
1:E:387:LEU:HD22	1:E:422:ILE:HG21	1.96	0.47
1:C:387:LEU:HD22	1:C:422:ILE:HG21	1.96	0.47
1:F:387:LEU:HD22	1:F:422:ILE:HG21	1.96	0.47
1:E:337:GLU:N	1:E:372:GLU:O	2.50	0.45
1:D:315:LEU:HD12	1:E:305:LEU:HD12	1.99	0.44
1:B:358:LEU:HD12	1:B:358:LEU:HA	1.84	0.44
1:C:315:LEU:HD12	1:D:305:LEU:HD12	1.98	0.44
1:C:337:GLU:N	1:C:372:GLU:O	2.50	0.44
1:B:337:GLU:N	1:B:372:GLU:O	2.50	0.44
1:E:367:VAL:HA	1:E:368:PRO:HD3	1.85	0.44
1:A:164:HIS:CD2	1:A:204:ASP:HB3	2.53	0.43
1:B:367:VAL:HA	1:B:368:PRO:HD3	1.85	0.43
1:D:164:HIS:CD2	1:D:204:ASP:HB3	2.53	0.43
1:C:164:HIS:CD2	1:C:204:ASP:HB3	2.54	0.43
1:F:367:VAL:HA	1:F:368:PRO:HD3	1.85	0.43
1:A:305:LEU:HD12	1:F:315:LEU:HD12	1.99	0.43
1:F:164:HIS:CD2	1:F:204:ASP:HB3	2.54	0.43
1:F:337:GLU:N	1:F:372:GLU:O	2.50	0.43
1:A:315:LEU:HD12	1:B:305:LEU:HD12	1.99	0.43
1:B:315:LEU:HD12	1:C:305:LEU:HD12	2.00	0.43
1:B:164:HIS:CD2	1:B:204:ASP:HB3	2.54	0.43
1:E:346:PRO:HG3	1:E:361:GLY:HA2	2.02	0.42
1:E:315:LEU:HD12	1:F:305:LEU:HD12	2.01	0.42
1:F:346:PRO:HG3	1:F:361:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:GLU:N	1:D:372:GLU:O	2.50	0.42
1:D:346:PRO:HG3	1:D:361:GLY:HA2	2.02	0.42
1:E:164:HIS:CD2	1:E:204:ASP:HB3	2.54	0.42
1:F:339:THR:HG23	1:F:368:PRO:HA	2.02	0.42
1:C:339:THR:HG23	1:C:368:PRO:HA	2.02	0.42
1:A:346:PRO:HG3	1:A:361:GLY:HA2	2.01	0.42
1:B:446:LYS:O	1:B:489:GLY:N	2.53	0.41
1:D:339:THR:HG23	1:D:368:PRO:HA	2.02	0.41
1:C:346:PRO:HG3	1:C:361:GLY:HA2	2.01	0.41
1:B:346:PRO:HG3	1:B:361:GLY:HA2	2.02	0.41
1:F:215:VAL:HG12	1:F:262:ALA:HB3	2.02	0.41
1:E:339:THR:HG23	1:E:368:PRO:HA	2.02	0.41
1:E:446:LYS:O	1:E:489:GLY:N	2.53	0.41
1:A:215:VAL:HG12	1:A:262:ALA:HB3	2.02	0.41
1:F:358:LEU:HA	1:F:358:LEU:HD12	1.84	0.41
1:A:339:THR:HG23	1:A:368:PRO:HA	2.02	0.41
1:D:178:LEU:HD21	1:D:185:PRO:HB3	2.03	0.41
1:A:446:LYS:O	1:A:489:GLY:N	2.53	0.41
1:B:339:THR:HG23	1:B:368:PRO:HA	2.02	0.41
1:B:411:LEU:HD21	1:B:483:ILE:HD11	2.03	0.41
1:B:472:SER:H	1:B:475:GLU:HB2	1.86	0.41
1:C:446:LYS:O	1:C:489:GLY:N	2.53	0.41
1:D:358:LEU:HA	1:D:358:LEU:HD12	1.84	0.41
1:E:215:VAL:HG12	1:E:262:ALA:HB3	2.02	0.41
1:F:446:LYS:O	1:F:489:GLY:N	2.53	0.41
1:A:411:LEU:HD21	1:A:483:ILE:HD11	2.03	0.41
1:D:215:VAL:HG12	1:D:262:ALA:HB3	2.02	0.41
1:D:446:LYS:O	1:D:489:GLY:N	2.53	0.41
1:A:456:ARG:NH1	1:A:499:ALA:O	2.54	0.40
1:B:215:VAL:HG12	1:B:262:ALA:HB3	2.02	0.40
1:C:472:SER:H	1:C:475:GLU:HB2	1.86	0.40
1:F:456:ARG:NH1	1:F:499:ALA:O	2.54	0.40
1:B:456:ARG:NH1	1:B:499:ALA:O	2.55	0.40
1:C:358:LEU:HA	1:C:358:LEU:HD12	1.84	0.40
1:F:294:THR:HB	1:F:297:SER:HB2	2.04	0.40
1:A:472:SER:H	1:A:475:GLU:HB2	1.86	0.40
1:E:178:LEU:HD21	1:E:185:PRO:HB3	2.03	0.40
1:E:294:THR:HB	1:E:297:SER:HB2	2.04	0.40
1:A:337:GLU:N	1:A:372:GLU:O	2.50	0.40
1:A:454:ASN:ND2	1:A:482:ARG:HB2	2.37	0.40
1:D:454:ASN:ND2	1:D:482:ARG:HB2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ASN:ND2	1:C:482:ARG:HB2	2.37	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	A	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	B	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	C	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	D	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	E	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
1	F	349/832 (42%)	345 (99%)	4 (1%)	0	100	100
All	All	2094/4992 (42%)	2070 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	293/683 (43%)	293 (100%)	0	100	100
1	B	293/683 (43%)	293 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	293/683 (43%)	293 (100%)	0	100	100
1	D	293/683 (43%)	293 (100%)	0	100	100
1	E	293/683 (43%)	293 (100%)	0	100	100
1	F	293/683 (43%)	293 (100%)	0	100	100
All	All	1758/4098 (43%)	1758 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	316	ASN
1	A	345	ASN
1	A	354	ASN
1	A	440	GLN
1	B	164	HIS
1	B	316	ASN
1	B	345	ASN
1	B	354	ASN
1	B	440	GLN
1	C	164	HIS
1	C	316	ASN
1	C	345	ASN
1	C	354	ASN
1	C	440	GLN
1	D	164	HIS
1	D	316	ASN
1	D	345	ASN
1	D	354	ASN
1	D	440	GLN
1	E	164	HIS
1	E	316	ASN
1	E	345	ASN
1	E	354	ASN
1	E	440	GLN
1	F	164	HIS
1	F	316	ASN
1	F	345	ASN
1	F	354	ASN

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Mol	Chain	Res	Type
1	F	440	GLN

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

This section contains visualisations of the EMDB entry EMD-20996. These allow visual inspection of the internal detail of the map and identification of artifacts.

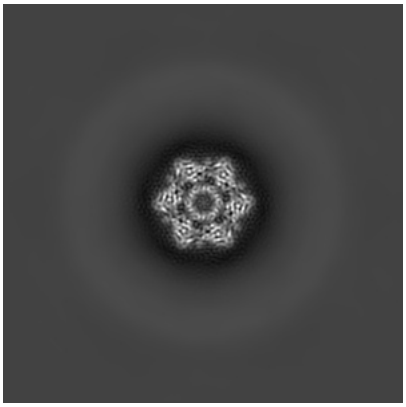
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

X

Y



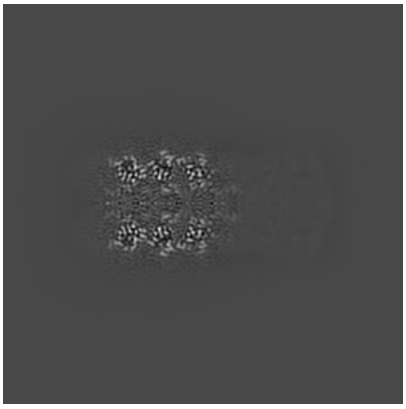
Z

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

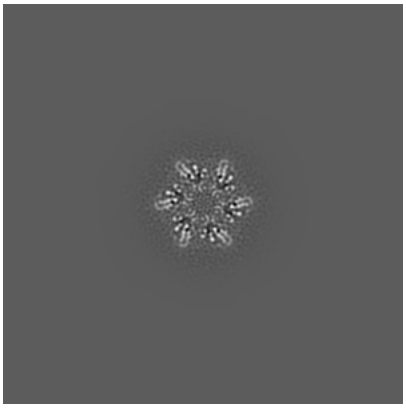
6.2 Central slices

6.2.1 Primary map

X Index: 140



Y Index: 140



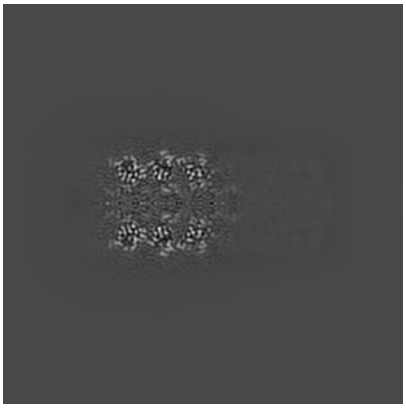
Z Index: 140

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

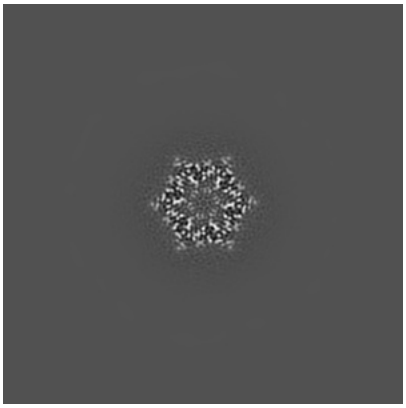
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 150



Y Index: 140

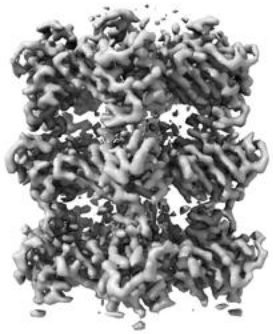


Z Index: 113

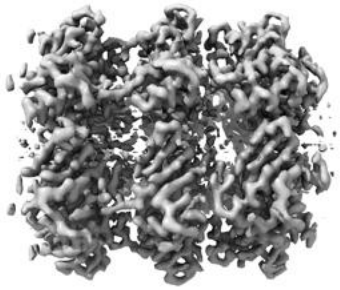
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

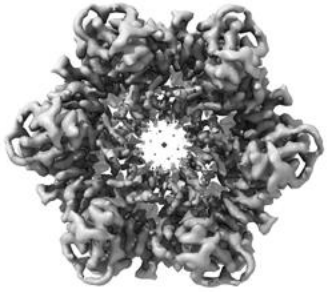
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

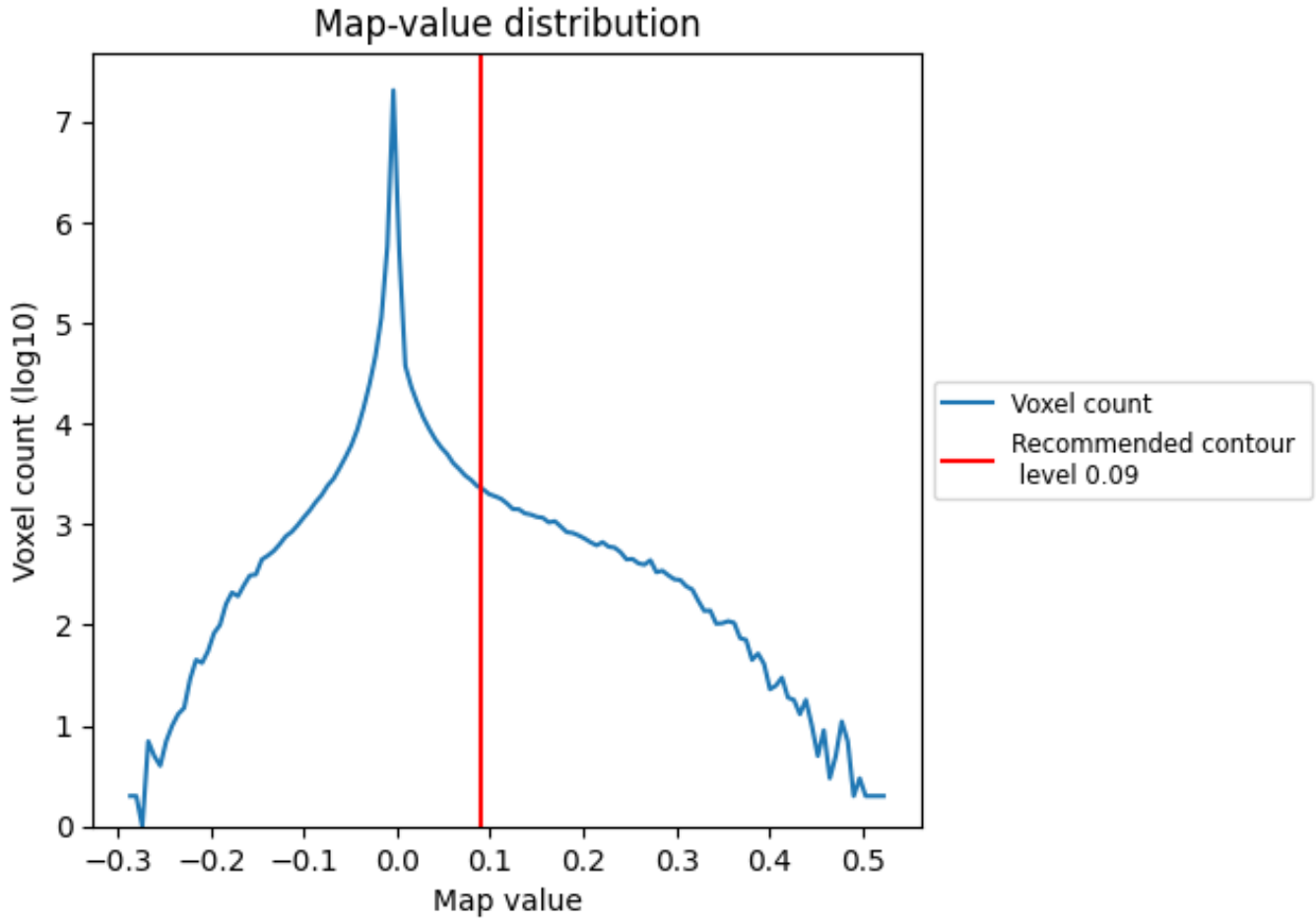
6.5 Mask visualisation (i)

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

7 Map analysis

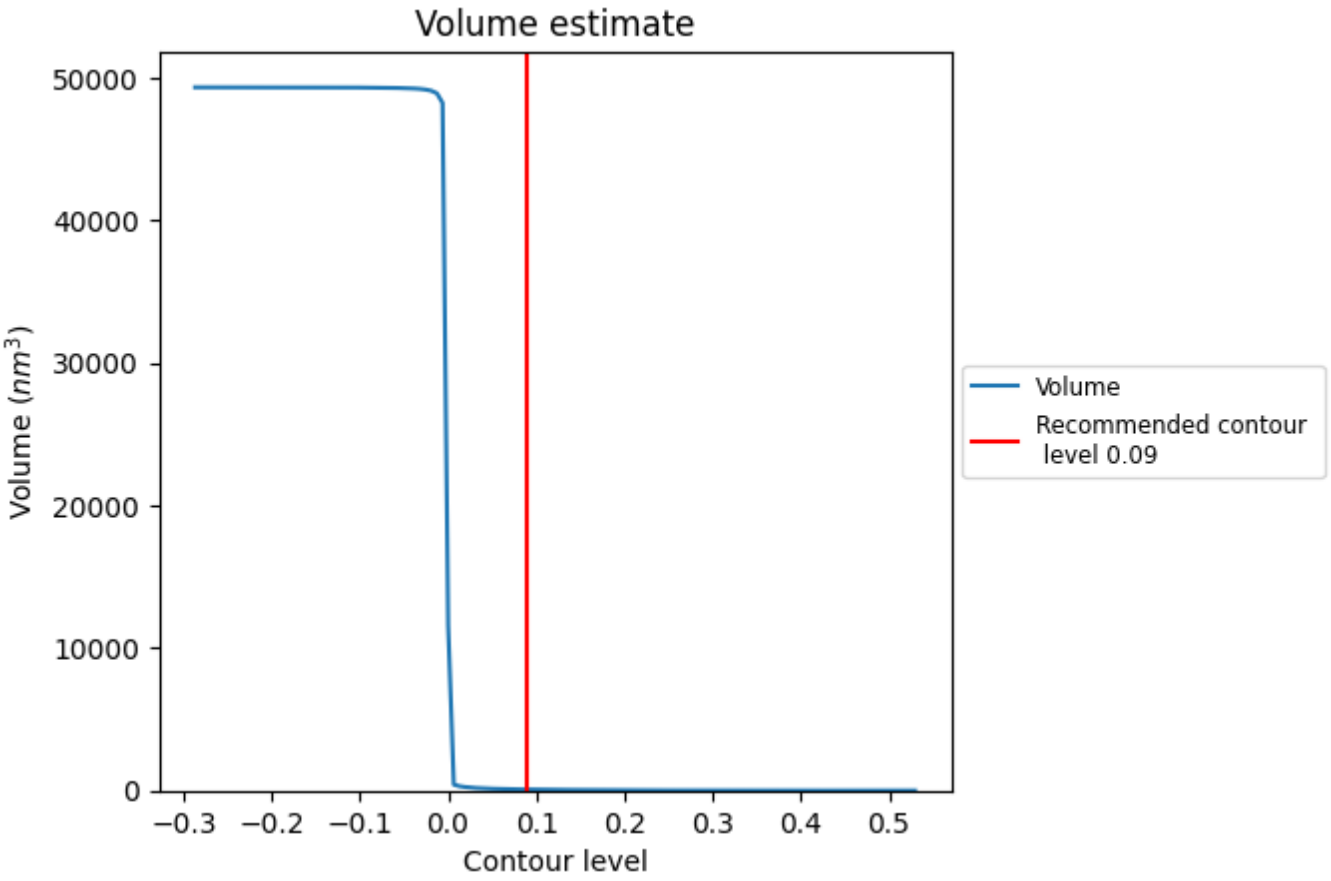
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

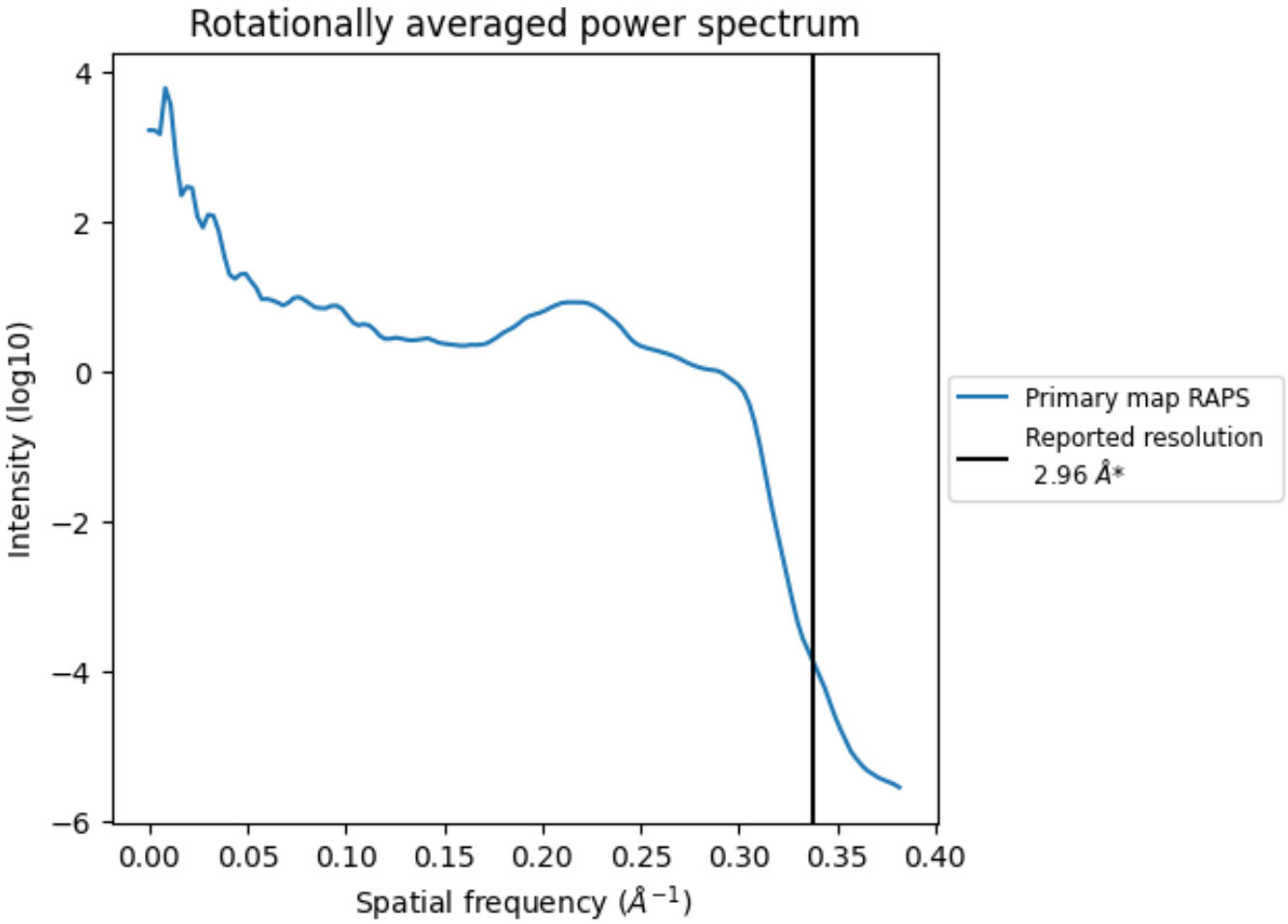
7.2 Volume estimate



The volume at the recommended contour level is 75 nm^3; this corresponds to an approximate mass of 68 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 0.338 Å^{-1}

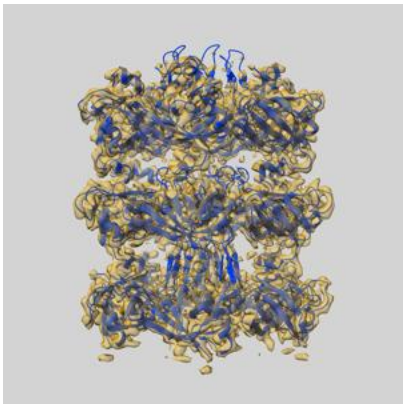
8 Fourier-Shell correlation (i)

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

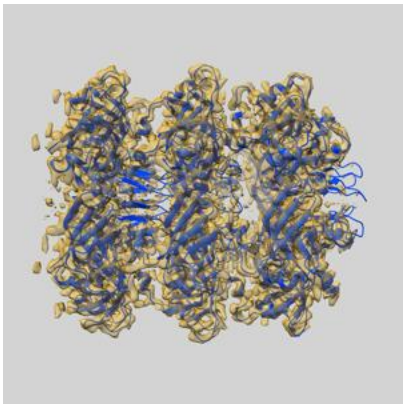
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20996 and PDB model 6V0F. Per-residue inclusion information can be found in section 3 on page 4.

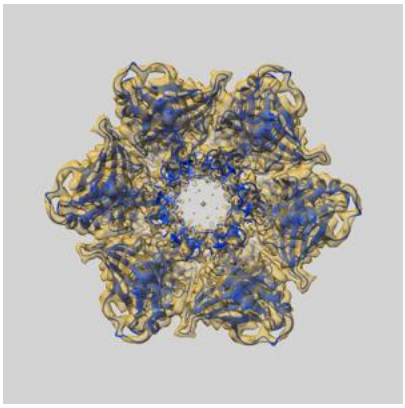
9.1 Map-model overlay



X



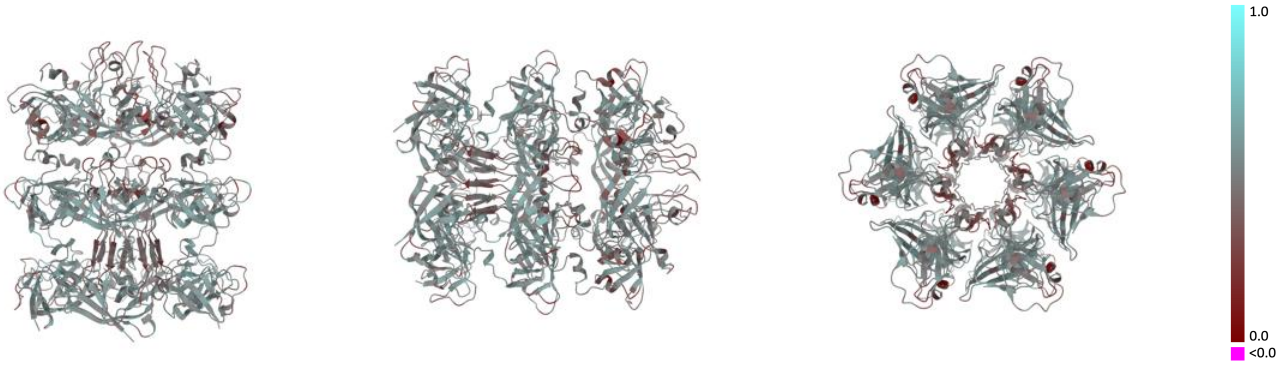
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

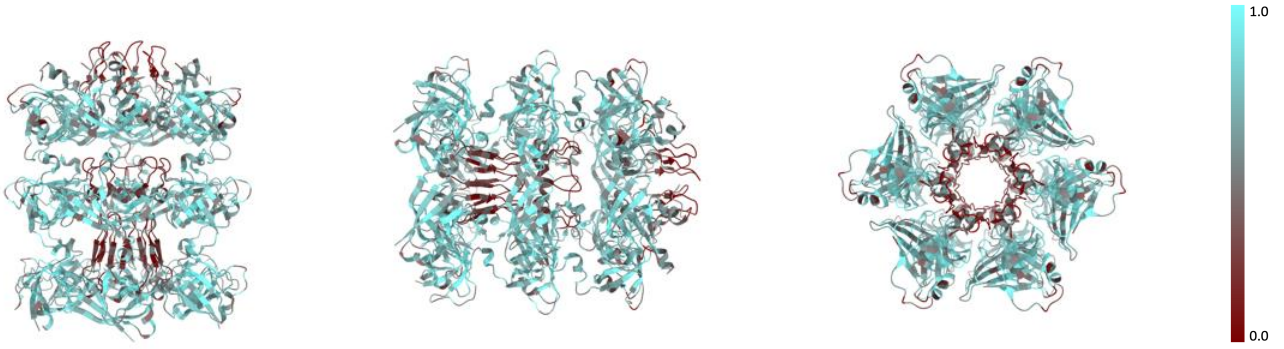
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

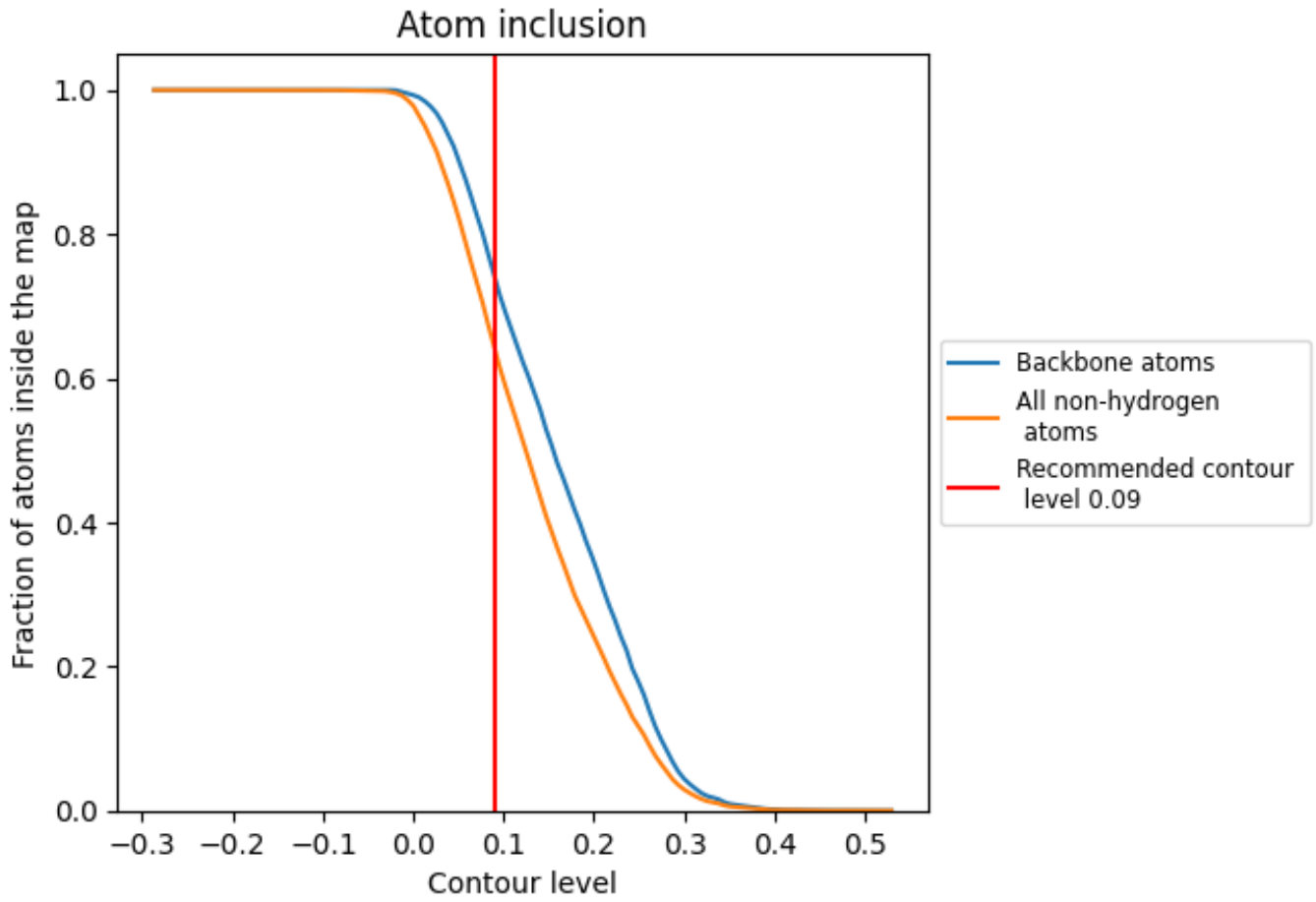
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6419	0.4860
A	0.6406	0.4880
B	0.6417	0.4840
C	0.6395	0.4860
D	0.6410	0.4860
E	0.6440	0.4840
F	0.6448	0.4890