Full wwPDB EM Validation Report

Mar 30, 2025 – 04:51 am BST

PDB ID	:	9EUI / pdb_00009eui
EMDB ID	:	EMD-19971
Title	:	Cryo-EM structure of Staphylococcus aureus bacteriophage phi812 baseplate in the post-contraction state - complete
Authors	:	Binovsky, J.; Siborova, M.; Baska, R.; Pichel-Beleiro, A.; Skubnik, K.; Novacek, J.; van Raaij, M.J.; Plevka, P.
Deposited on	:	2024-03-27
Resolution	:	4.40 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 (i) 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 (i)) were used in the production of this report:

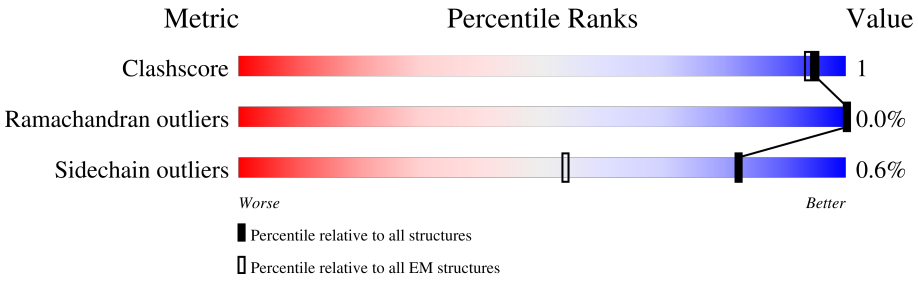
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	234	95%
2	B	348	97%
2	C	348	95%
3	D	1019	5% 36% 63%
4	E	587	86% 6% 8%
4	F	587	89% 5% 6%
4	G	587	6% 89% 5% 6%
4	H	587	6% 90% 6%

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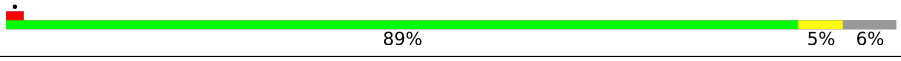
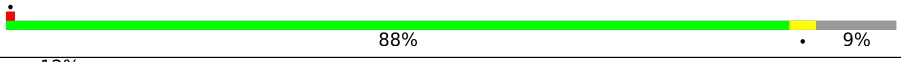
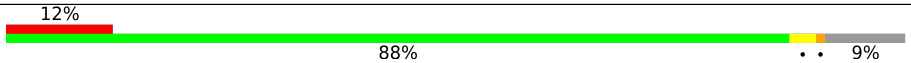
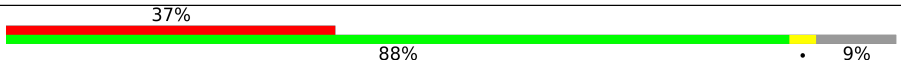
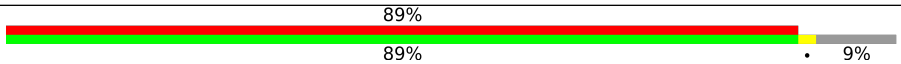
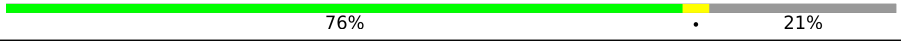
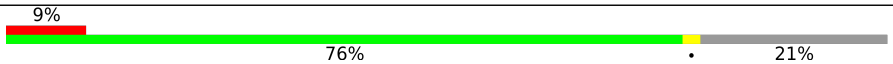
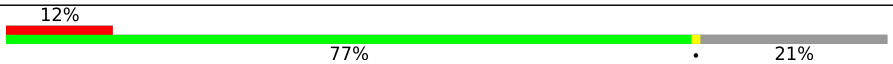
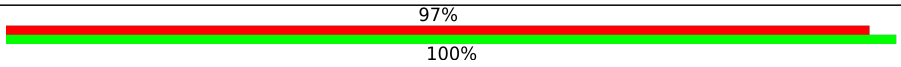
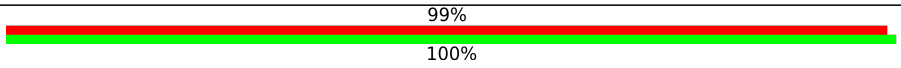
Mol	Chain	Length	Quality of chain
4	I	587	
4	J	587	
5	K	194	
5	L	194	
5	M	194	
5	N	194	
5	O	194	
5	P	194	
6	Q	1152	
6	R	1152	
6	S	1152	
6	T	1152	
6	U	1152	
6	V	1152	
7	W	458	
7	X	458	
7	Y	458	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 92215 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 Baseplate wedge subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	234	Total	C	N	O	S	0	0
			1871	1174	314	377	6		

- Molecule 2 is a protein called Baseplate component.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
2	C	347	Total	C	N	O	S	0	0
			2752	1729	458	559	6		

- Molecule 3 is a protein called TmpF.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	373	Total	C	N	O	S	0	0
			2252	1333	438	479	2		

- Molecule 4 is a protein called Major tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	540	Total	C	N	O	S	0	0
			4213	2653	714	839	7		
4	F	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
4	G	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
4	H	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
4	I	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
4	J	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		

- Molecule 5 is a protein called Baseplate protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	176	Total	C	N	O	S	0	0
			1378	874	226	277	1		
5	L	176	Total	C	N	O	S	0	0
			1378	874	226	277	1		
5	M	176	Total	C	N	O	S	0	0
			1378	874	226	277	1		
5	N	176	Total	C	N	O	S	0	0
			1378	874	226	277	1		
5	O	176	Total	C	N	O	S	0	0
			1378	874	226	277	1		
5	P	176	Total	C	N	O	S	0	0
			1378	874	226	277	1		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	174	ASP	-	expression tag	UNP A0A0U1WGQ5
K	175	PRO	-	expression tag	UNP A0A0U1WGQ5
K	176	ASN	-	expression tag	UNP A0A0U1WGQ5
K	177	SER	-	expression tag	UNP A0A0U1WGQ5
K	178	SER	-	expression tag	UNP A0A0U1WGQ5
K	179	SER	-	expression tag	UNP A0A0U1WGQ5
K	180	VAL	-	expression tag	UNP A0A0U1WGQ5
K	181	ASP	-	expression tag	UNP A0A0U1WGQ5
K	182	LYS	-	expression tag	UNP A0A0U1WGQ5
K	183	LEU	-	expression tag	UNP A0A0U1WGQ5
K	184	ALA	-	expression tag	UNP A0A0U1WGQ5
K	185	ALA	-	expression tag	UNP A0A0U1WGQ5
K	186	ALA	-	expression tag	UNP A0A0U1WGQ5
K	187	LEU	-	expression tag	UNP A0A0U1WGQ5
K	188	GLU	-	expression tag	UNP A0A0U1WGQ5
K	189	HIS	-	expression tag	UNP A0A0U1WGQ5
K	190	HIS	-	expression tag	UNP A0A0U1WGQ5
K	191	HIS	-	expression tag	UNP A0A0U1WGQ5
K	192	HIS	-	expression tag	UNP A0A0U1WGQ5
K	193	HIS	-	expression tag	UNP A0A0U1WGQ5
K	194	HIS	-	expression tag	UNP A0A0U1WGQ5
L	174	ASP	-	expression tag	UNP A0A0U1WGQ5
L	175	PRO	-	expression tag	UNP A0A0U1WGQ5
L	176	ASN	-	expression tag	UNP A0A0U1WGQ5
L	177	SER	-	expression tag	UNP A0A0U1WGQ5
L	178	SER	-	expression tag	UNP A0A0U1WGQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
L	179	SER	-	expression tag	UNP A0A0U1WGQ5
L	180	VAL	-	expression tag	UNP A0A0U1WGQ5
L	181	ASP	-	expression tag	UNP A0A0U1WGQ5
L	182	LYS	-	expression tag	UNP A0A0U1WGQ5
L	183	LEU	-	expression tag	UNP A0A0U1WGQ5
L	184	ALA	-	expression tag	UNP A0A0U1WGQ5
L	185	ALA	-	expression tag	UNP A0A0U1WGQ5
L	186	ALA	-	expression tag	UNP A0A0U1WGQ5
L	187	LEU	-	expression tag	UNP A0A0U1WGQ5
L	188	GLU	-	expression tag	UNP A0A0U1WGQ5
L	189	HIS	-	expression tag	UNP A0A0U1WGQ5
L	190	HIS	-	expression tag	UNP A0A0U1WGQ5
L	191	HIS	-	expression tag	UNP A0A0U1WGQ5
L	192	HIS	-	expression tag	UNP A0A0U1WGQ5
L	193	HIS	-	expression tag	UNP A0A0U1WGQ5
L	194	HIS	-	expression tag	UNP A0A0U1WGQ5
M	174	ASP	-	expression tag	UNP A0A0U1WGQ5
M	175	PRO	-	expression tag	UNP A0A0U1WGQ5
M	176	ASN	-	expression tag	UNP A0A0U1WGQ5
M	177	SER	-	expression tag	UNP A0A0U1WGQ5
M	178	SER	-	expression tag	UNP A0A0U1WGQ5
M	179	SER	-	expression tag	UNP A0A0U1WGQ5
M	180	VAL	-	expression tag	UNP A0A0U1WGQ5
M	181	ASP	-	expression tag	UNP A0A0U1WGQ5
M	182	LYS	-	expression tag	UNP A0A0U1WGQ5
M	183	LEU	-	expression tag	UNP A0A0U1WGQ5
M	184	ALA	-	expression tag	UNP A0A0U1WGQ5
M	185	ALA	-	expression tag	UNP A0A0U1WGQ5
M	186	ALA	-	expression tag	UNP A0A0U1WGQ5
M	187	LEU	-	expression tag	UNP A0A0U1WGQ5
M	188	GLU	-	expression tag	UNP A0A0U1WGQ5
M	189	HIS	-	expression tag	UNP A0A0U1WGQ5
M	190	HIS	-	expression tag	UNP A0A0U1WGQ5
M	191	HIS	-	expression tag	UNP A0A0U1WGQ5
M	192	HIS	-	expression tag	UNP A0A0U1WGQ5
M	193	HIS	-	expression tag	UNP A0A0U1WGQ5
M	194	HIS	-	expression tag	UNP A0A0U1WGQ5
N	174	ASP	-	expression tag	UNP A0A0U1WGQ5
N	175	PRO	-	expression tag	UNP A0A0U1WGQ5
N	176	ASN	-	expression tag	UNP A0A0U1WGQ5
N	177	SER	-	expression tag	UNP A0A0U1WGQ5
N	178	SER	-	expression tag	UNP A0A0U1WGQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
N	179	SER	-	expression tag	UNP A0A0U1WGQ5
N	180	VAL	-	expression tag	UNP A0A0U1WGQ5
N	181	ASP	-	expression tag	UNP A0A0U1WGQ5
N	182	LYS	-	expression tag	UNP A0A0U1WGQ5
N	183	LEU	-	expression tag	UNP A0A0U1WGQ5
N	184	ALA	-	expression tag	UNP A0A0U1WGQ5
N	185	ALA	-	expression tag	UNP A0A0U1WGQ5
N	186	ALA	-	expression tag	UNP A0A0U1WGQ5
N	187	LEU	-	expression tag	UNP A0A0U1WGQ5
N	188	GLU	-	expression tag	UNP A0A0U1WGQ5
N	189	HIS	-	expression tag	UNP A0A0U1WGQ5
N	190	HIS	-	expression tag	UNP A0A0U1WGQ5
N	191	HIS	-	expression tag	UNP A0A0U1WGQ5
N	192	HIS	-	expression tag	UNP A0A0U1WGQ5
N	193	HIS	-	expression tag	UNP A0A0U1WGQ5
N	194	HIS	-	expression tag	UNP A0A0U1WGQ5
O	174	ASP	-	expression tag	UNP A0A0U1WGQ5
O	175	PRO	-	expression tag	UNP A0A0U1WGQ5
O	176	ASN	-	expression tag	UNP A0A0U1WGQ5
O	177	SER	-	expression tag	UNP A0A0U1WGQ5
O	178	SER	-	expression tag	UNP A0A0U1WGQ5
O	179	SER	-	expression tag	UNP A0A0U1WGQ5
O	180	VAL	-	expression tag	UNP A0A0U1WGQ5
O	181	ASP	-	expression tag	UNP A0A0U1WGQ5
O	182	LYS	-	expression tag	UNP A0A0U1WGQ5
O	183	LEU	-	expression tag	UNP A0A0U1WGQ5
O	184	ALA	-	expression tag	UNP A0A0U1WGQ5
O	185	ALA	-	expression tag	UNP A0A0U1WGQ5
O	186	ALA	-	expression tag	UNP A0A0U1WGQ5
O	187	LEU	-	expression tag	UNP A0A0U1WGQ5
O	188	GLU	-	expression tag	UNP A0A0U1WGQ5
O	189	HIS	-	expression tag	UNP A0A0U1WGQ5
O	190	HIS	-	expression tag	UNP A0A0U1WGQ5
O	191	HIS	-	expression tag	UNP A0A0U1WGQ5
O	192	HIS	-	expression tag	UNP A0A0U1WGQ5
O	193	HIS	-	expression tag	UNP A0A0U1WGQ5
O	194	HIS	-	expression tag	UNP A0A0U1WGQ5
P	174	ASP	-	expression tag	UNP A0A0U1WGQ5
P	175	PRO	-	expression tag	UNP A0A0U1WGQ5
P	176	ASN	-	expression tag	UNP A0A0U1WGQ5
P	177	SER	-	expression tag	UNP A0A0U1WGQ5
P	178	SER	-	expression tag	UNP A0A0U1WGQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
P	179	SER	-	expression tag	UNP A0A0U1WGQ5
P	180	VAL	-	expression tag	UNP A0A0U1WGQ5
P	181	ASP	-	expression tag	UNP A0A0U1WGQ5
P	182	LYS	-	expression tag	UNP A0A0U1WGQ5
P	183	LEU	-	expression tag	UNP A0A0U1WGQ5
P	184	ALA	-	expression tag	UNP A0A0U1WGQ5
P	185	ALA	-	expression tag	UNP A0A0U1WGQ5
P	186	ALA	-	expression tag	UNP A0A0U1WGQ5
P	187	LEU	-	expression tag	UNP A0A0U1WGQ5
P	188	GLU	-	expression tag	UNP A0A0U1WGQ5
P	189	HIS	-	expression tag	UNP A0A0U1WGQ5
P	190	HIS	-	expression tag	UNP A0A0U1WGQ5
P	191	HIS	-	expression tag	UNP A0A0U1WGQ5
P	192	HIS	-	expression tag	UNP A0A0U1WGQ5
P	193	HIS	-	expression tag	UNP A0A0U1WGQ5
P	194	HIS	-	expression tag	UNP A0A0U1WGQ5

- Molecule 6 is a protein called DUF4815 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
6	R	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
6	S	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
6	T	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
6	U	908	Total	C	N	O	S	0	0
			7165	4510	1184	1453	18		
6	V	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		

- Molecule 7 is a protein called Receptor binding protein.

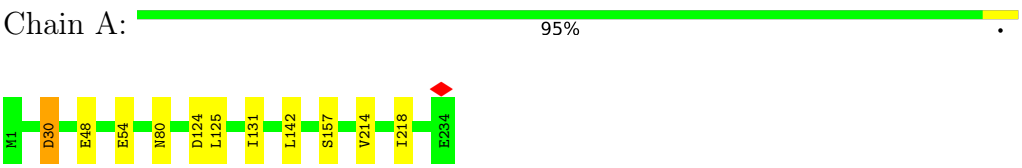
Mol	Chain	Residues	Atoms				AltConf	Trace
7	W	458	Total	C	N	O	0	0
			1833	916	458	459		
7	X	458	Total	C	N	O	0	0
			1833	916	458	459		
7	Y	458	Total	C	N	O	0	0
			1833	916	458	459		

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.

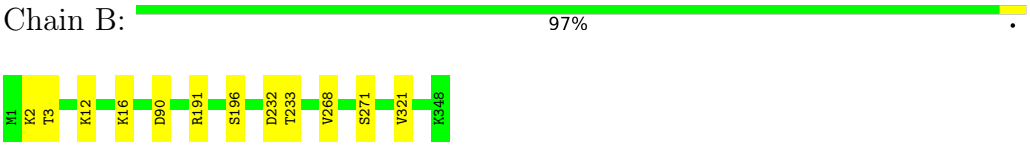
• Molecule 1: Baseplate wedge subunit

Chain A:



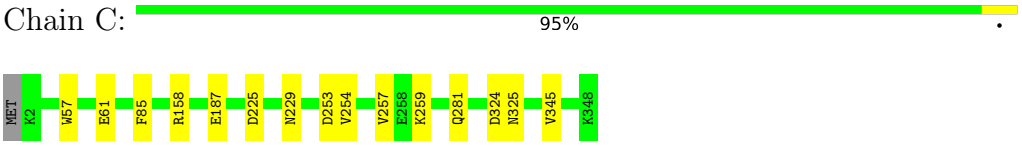
• Molecule 2: Baseplate component

Chain B:



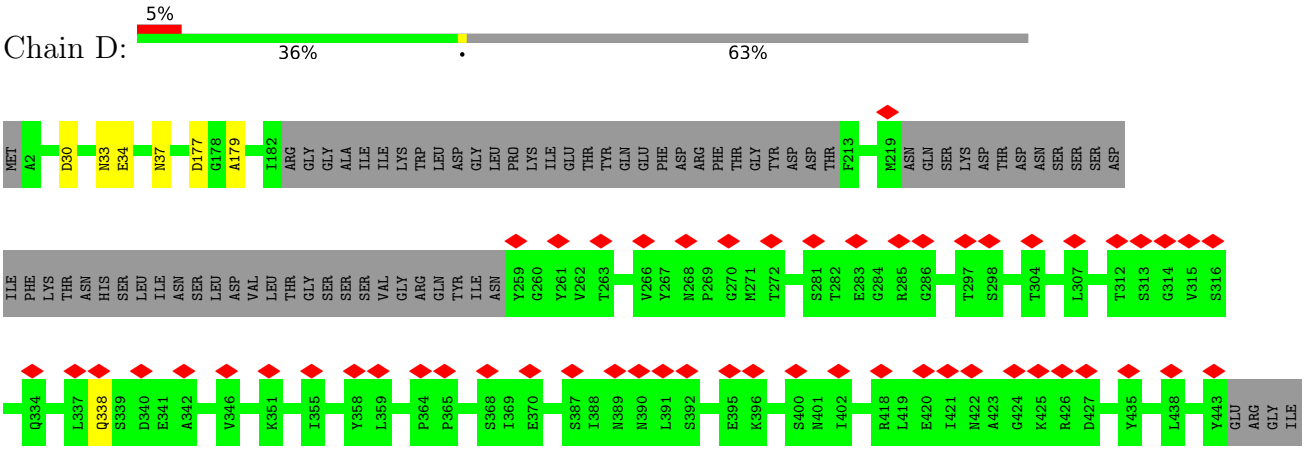
• Molecule 2: Baseplate component

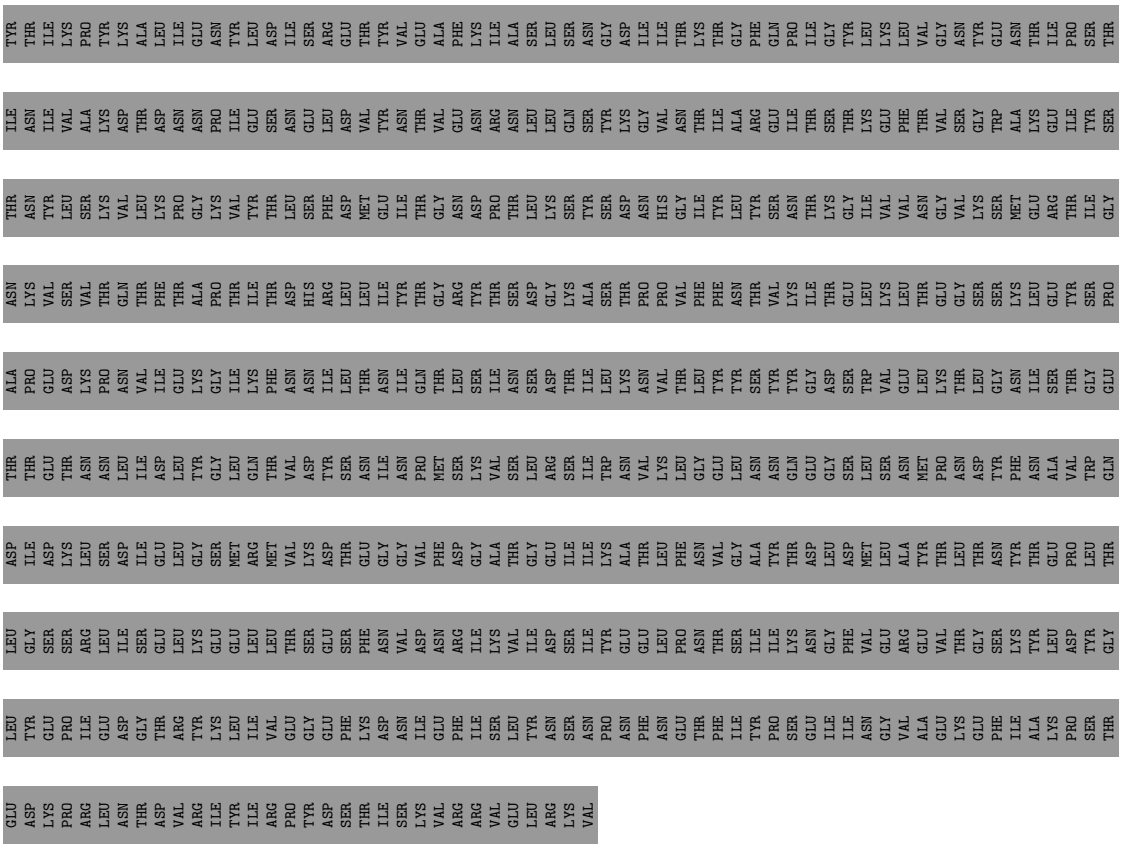
Chain C:



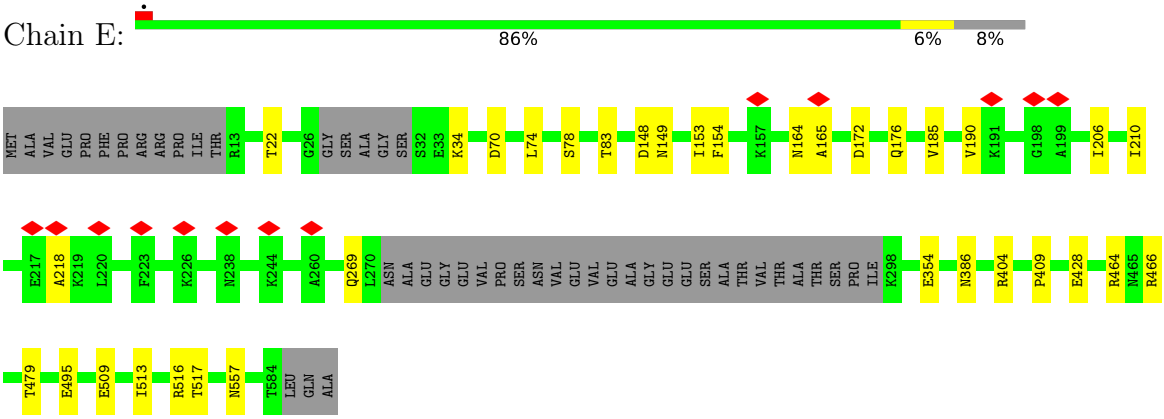
• Molecule 3: TmpF

Chain D:

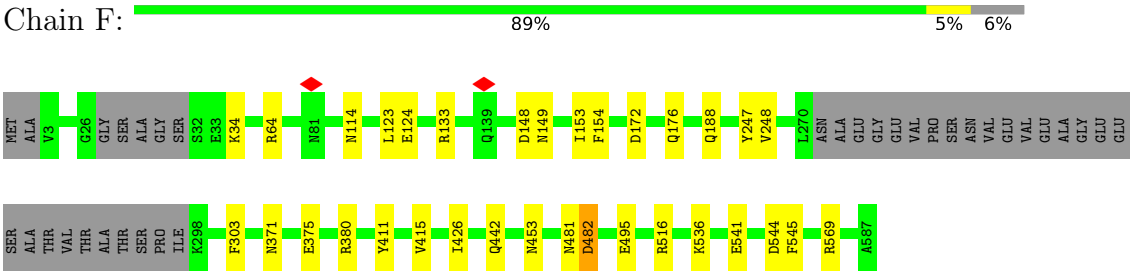




• Molecule 4: Major tail sheath protein

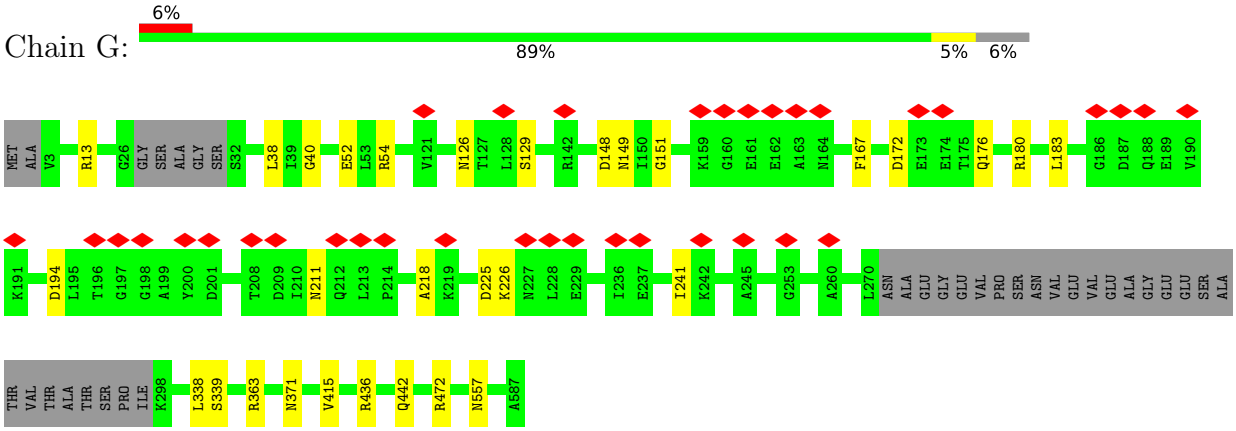


• Molecule 4: Major tail sheath protein



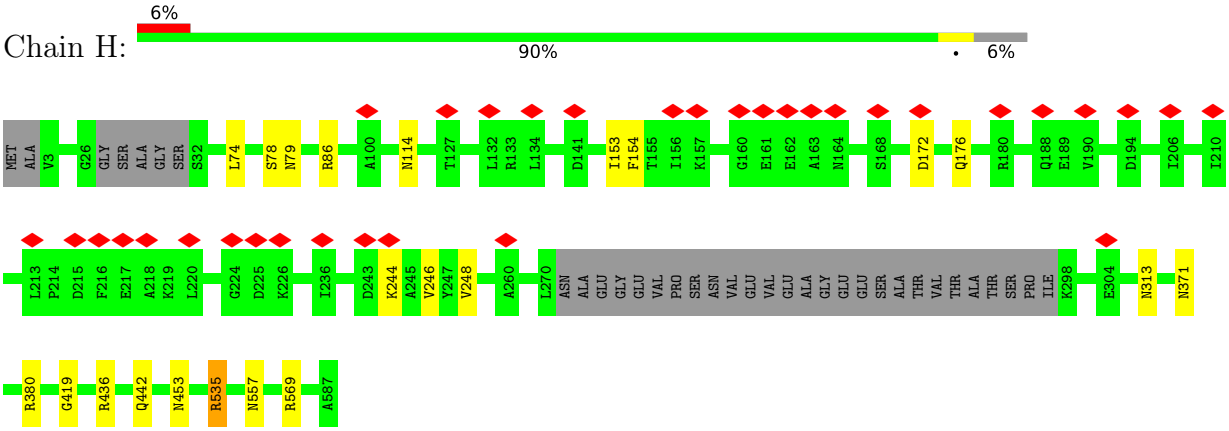
• Molecule 4: Major tail sheath protein

Chain G:



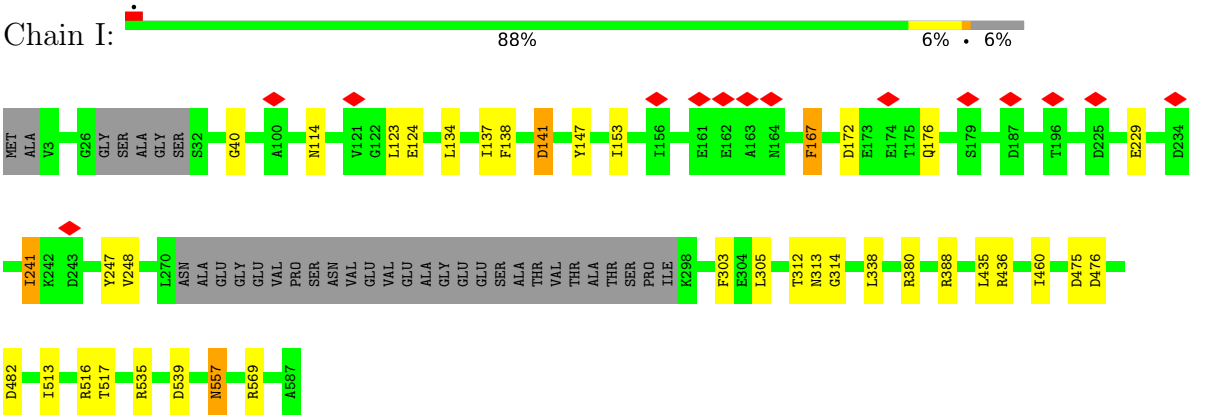
• Molecule 4: Major tail sheath protein

Chain H:



• Molecule 4: Major tail sheath protein

Chain I:



• Molecule 4: Major tail sheath protein

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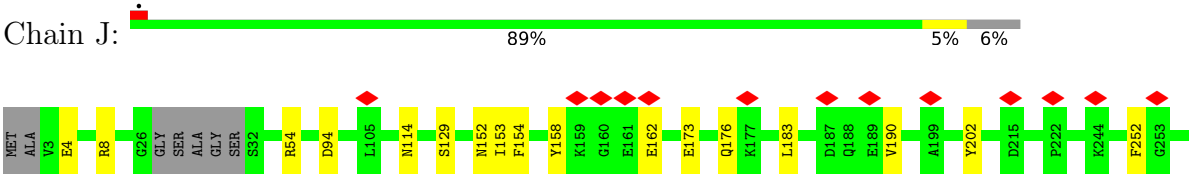
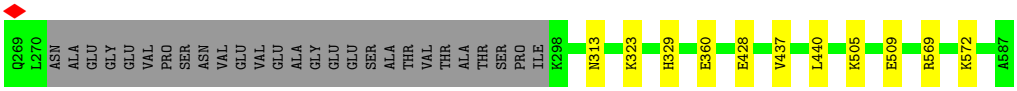
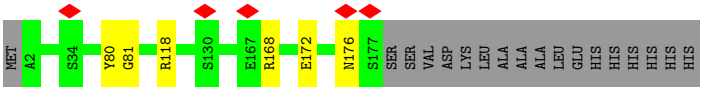




• Molecule 5: Baseplate protein

Chain K:



• Molecule 5: Baseplate protein

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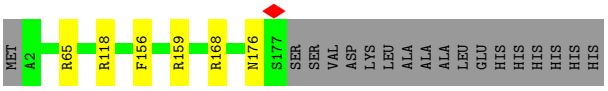
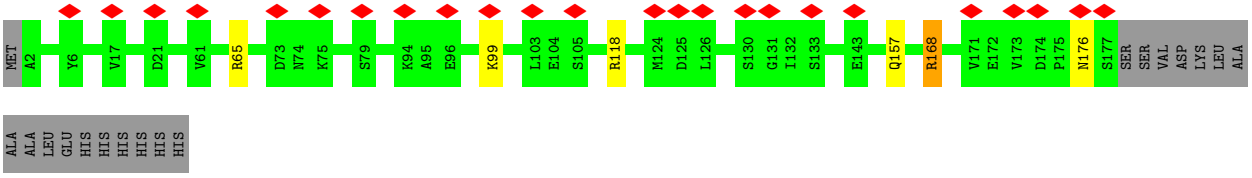


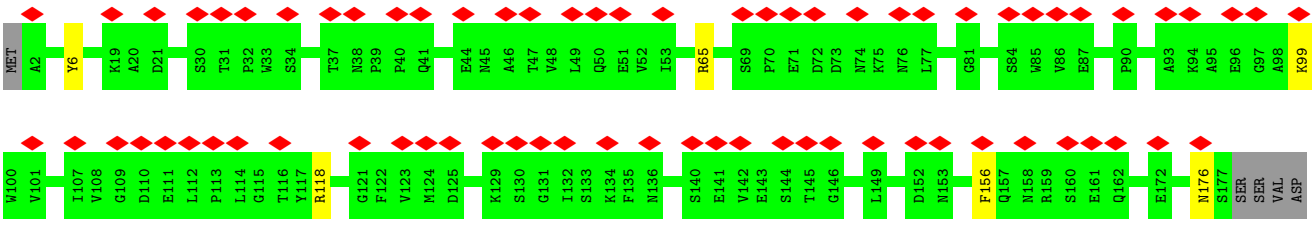
• Molecule 5: Baseplate protein

Chain M:



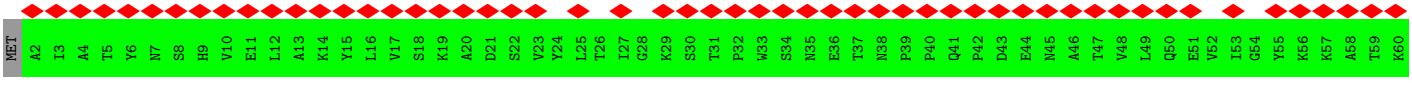
• Molecule 5: Baseplate protein

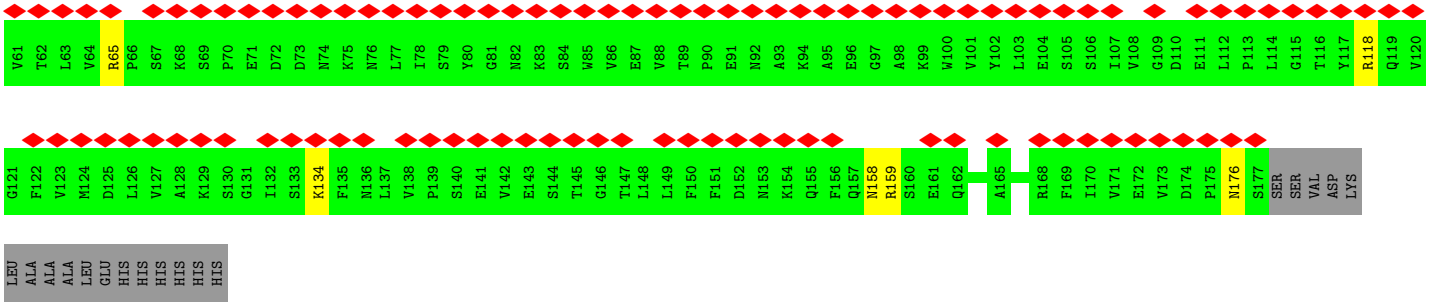
Chain N:



• Molecule 5: Baseplate protein

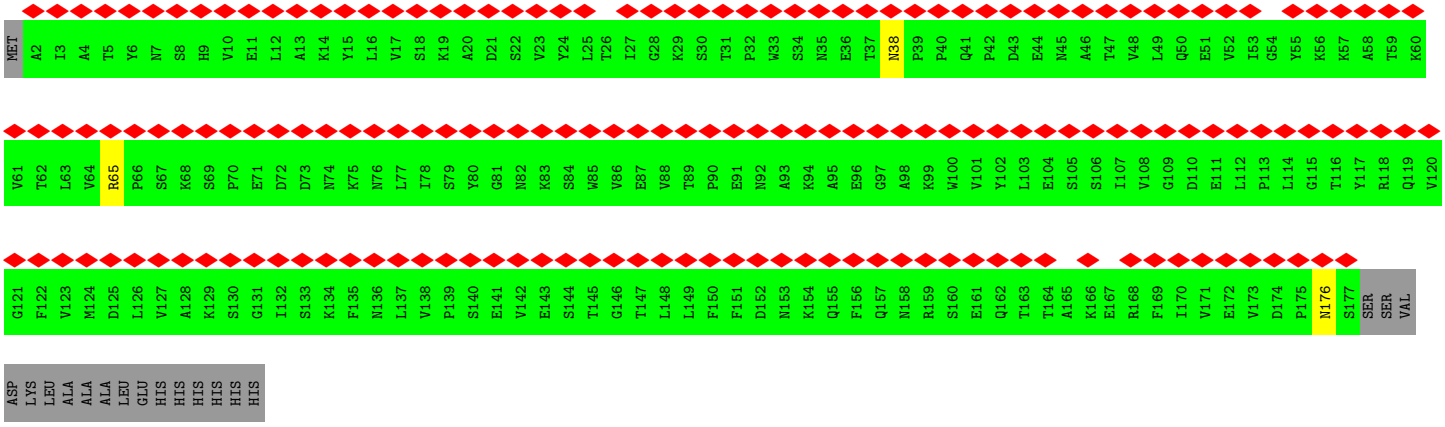
Chain O:





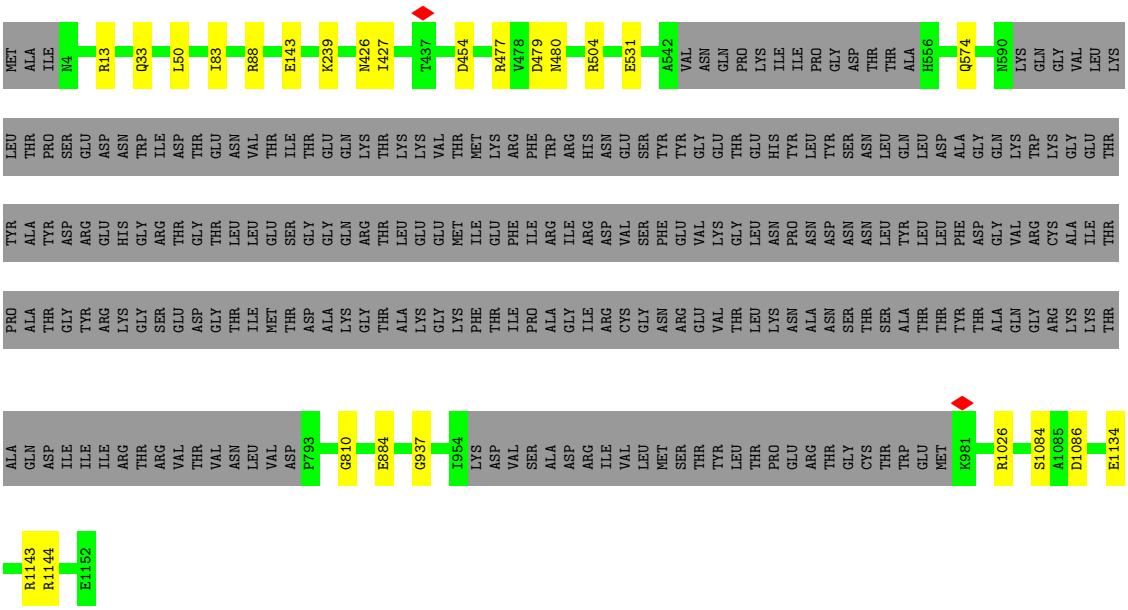
• Molecule 5: Baseplate protein

Chain P:



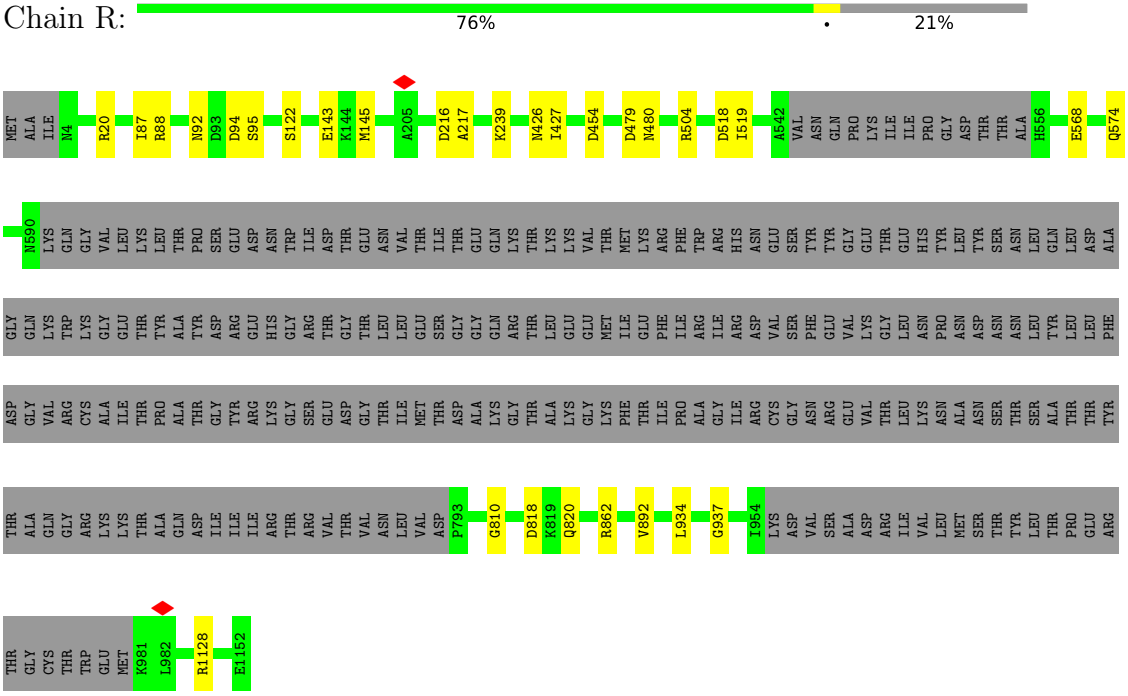
• Molecule 6: DUF4815 domain-containing protein

Chain Q:



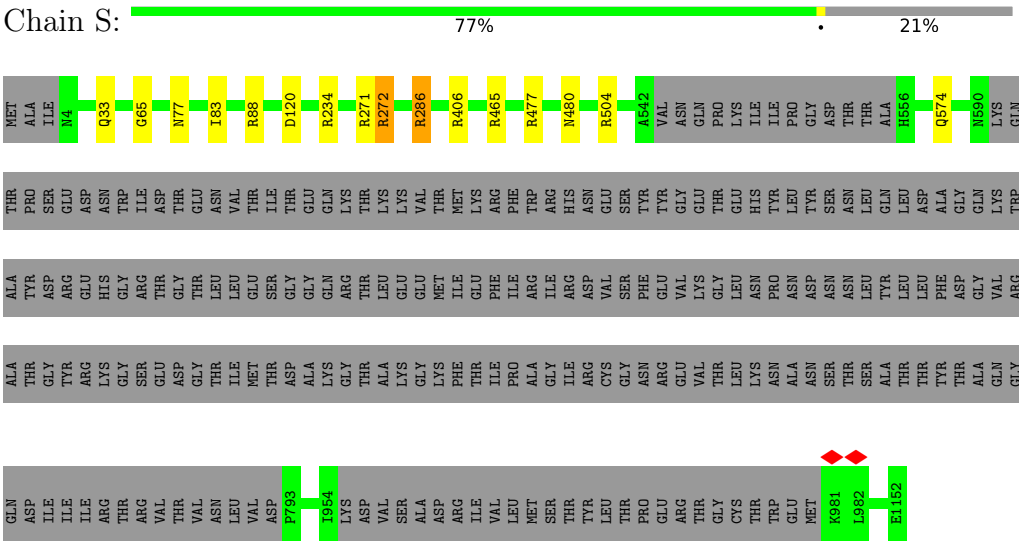
• Molecule 6: DUF4815 domain-containing protein

Chain R:



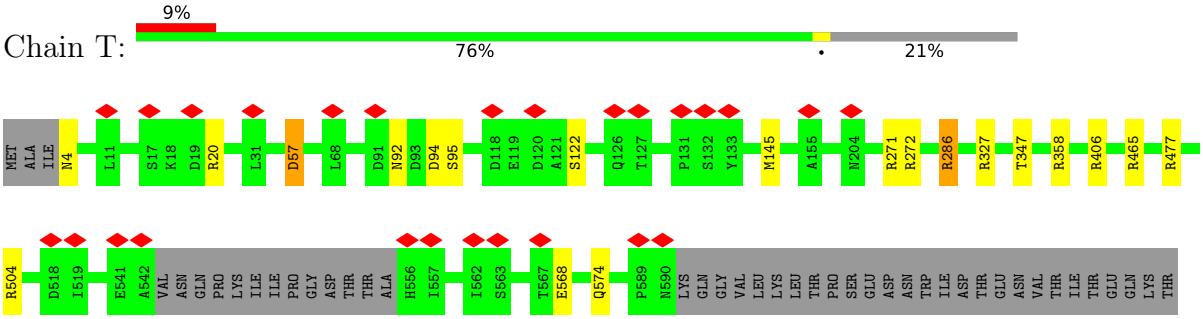
• Molecule 6: DUF4815 domain-containing protein

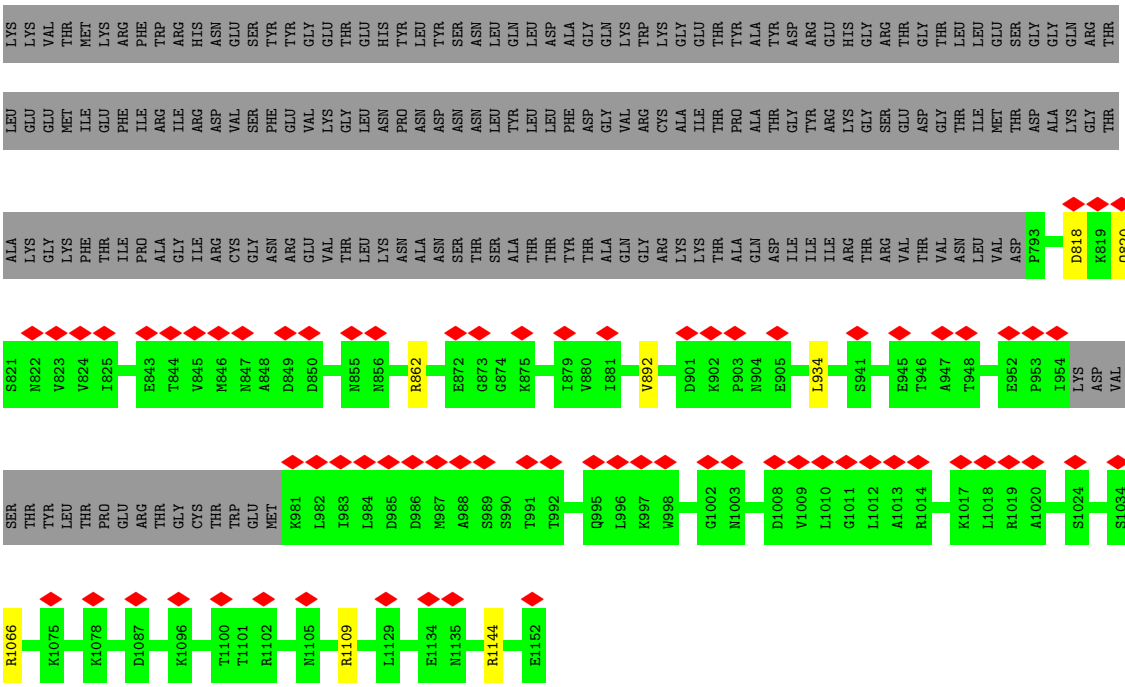
Chain S:



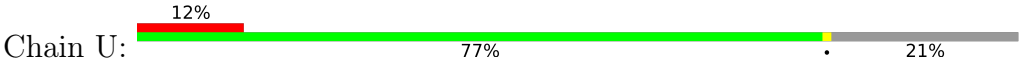
• Molecule 6: DUF4815 domain-containing protein

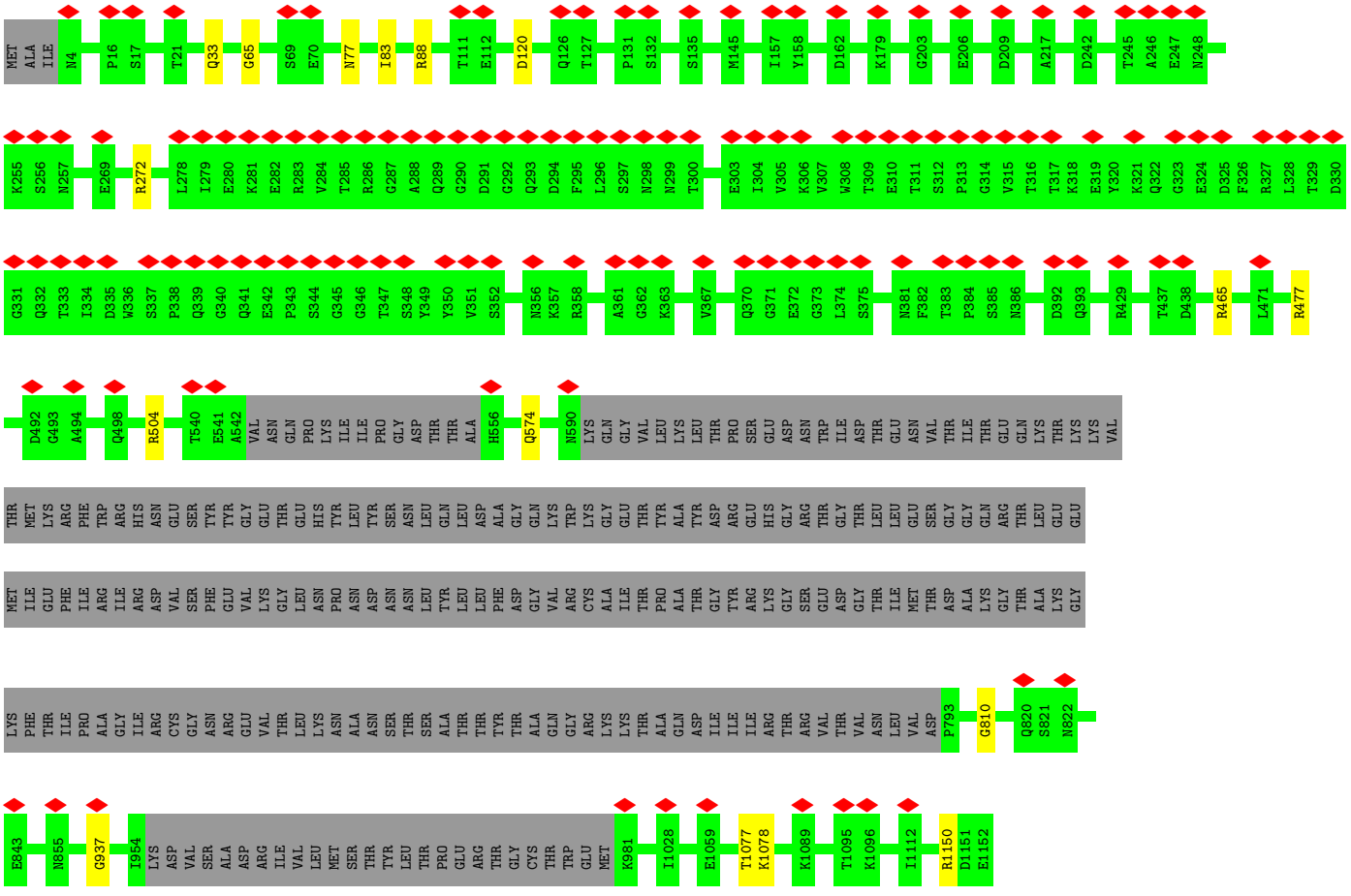
Chain T:





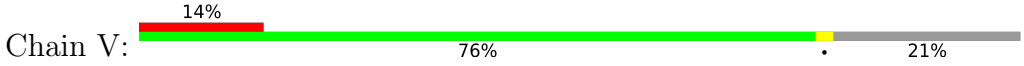
• Molecule 6: DUF4815 domain-containing protein

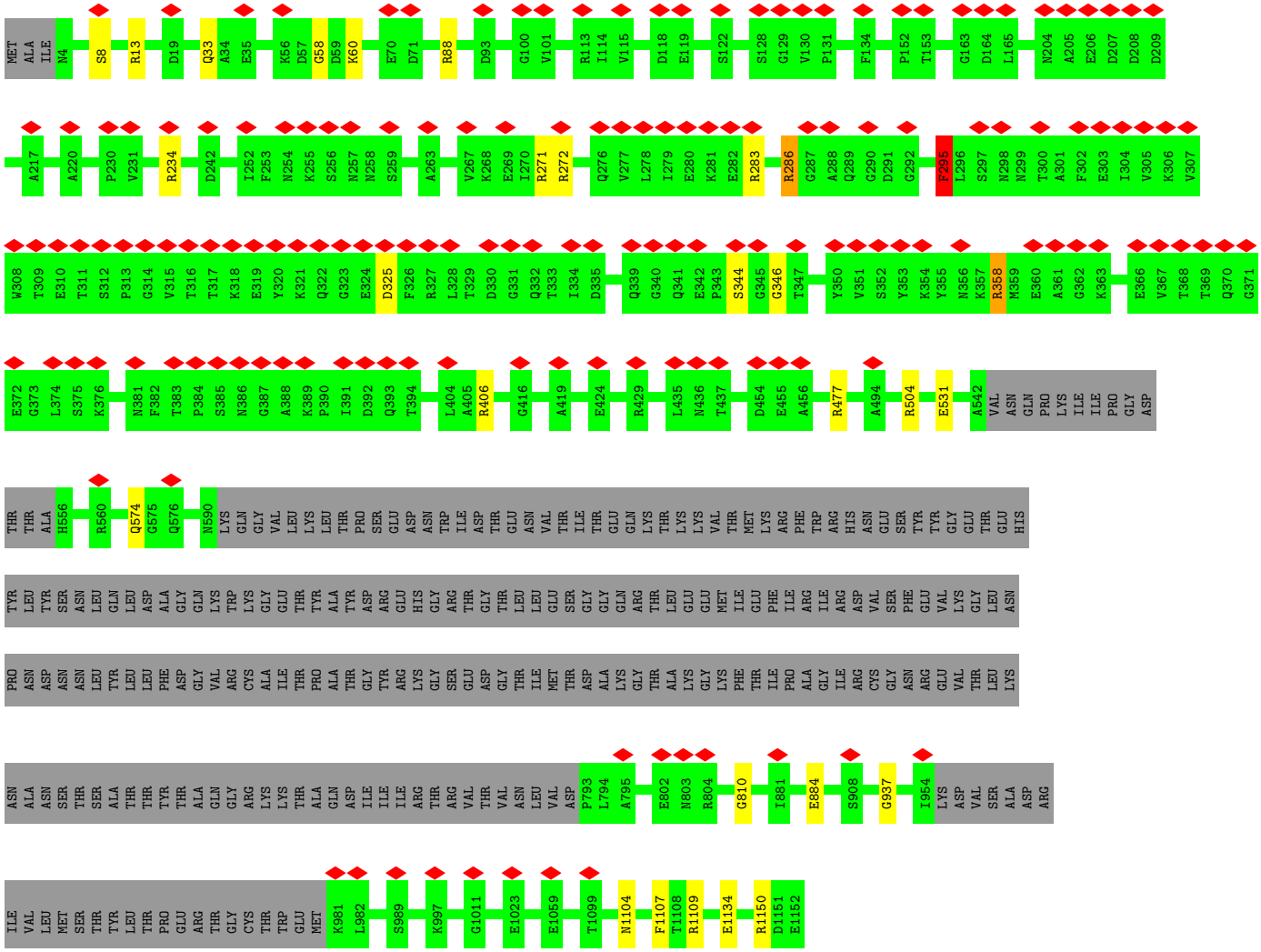




• Molecule 6: DUF4815 domain-containing protein

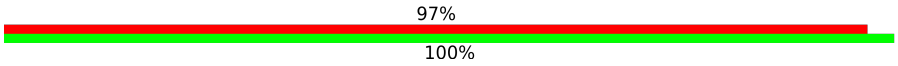
Chain V:

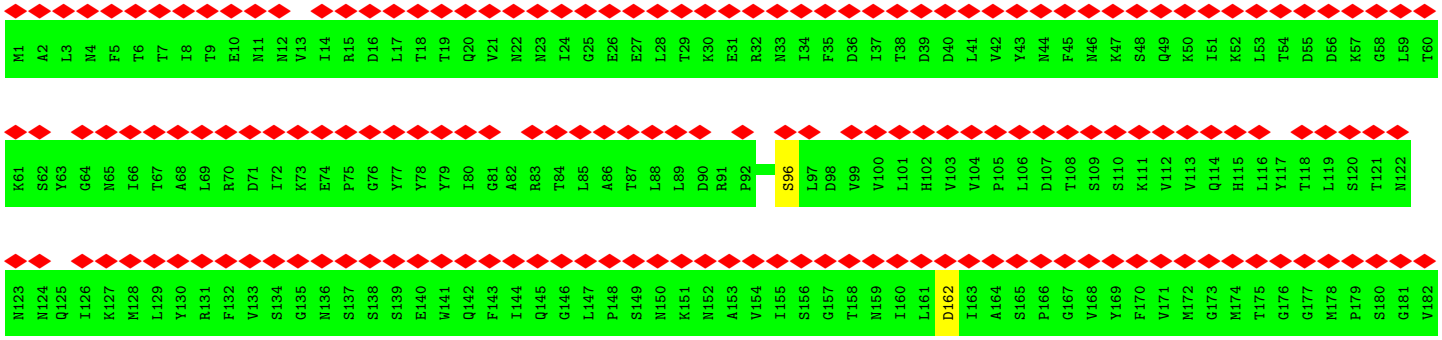




• Molecule 7: Receptor binding protein

Chain W:





S183 S184 G185 F186 L187 D188 L189 S190 V191 D192 A193 N194 D195 N196 R197 L198 A199 R200 L201 T202 D203 A204 E205 T206 G207 K208 E209 Y210 T211 S212 I213 K214 K215 P216 T217 G218 T219 Y220 T221 A222 W223 K224 K225 E226 F227 E228 P229 K230 D231 M232 E233 K234 Y235 L236 L237 S238 S239 I240 R241 D242

D243 G244 S245 A246 S247 F248 P249 L250 L251 V252 Y253 T254 S255 D256 S257 K258 T259 F260 Q261 Q262 A263 I264 I265 D266 H267 I268 D269 R270 T271 G272 Q273 T274 T275 F276 T277 F278 Y279 V280 Q281 G282 G283 V284 S285 G286 S287 P288 M289 S290 N291 S292 C293 R294 G295 L296 F297 M298 S299 D300 T301 P302

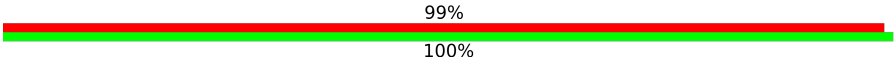
N303 T304 S305 S306 L307 H308 G309 V310 Y311 N312 A313 I314 G315 T316 D317 G318 R319 N320 V321 T322 G323 S324 V325 V326 G327 S328 N329 W330 T331 S332 P333 K334 T335 S336 P337 S338 H339 K340 E341 L342 W343 T344 G345 A346 Q347 S348 F349 L350 S351 T352 G353 T354 T355 K356 N357 L358 S359 D360 D361 I362

S363 N364 Y365 S366 Y367 V368 E369 V370 Y371 T372 T373 H374 K375 T376 T377 E378 K379 T380 K381 G382 N383 D384 N385 T386 G387 T388 I389 C390 H391 K392 F393 Y394 L395 D396 G397 S398 G399 T400 Y401 V402 C403 S404 G405 T406 F407 V408 S409 G410 D411 R412 T413 D414 T415 K416 P417 P418 I419 T420 E421 F422

Y423 R424 V425 G426 V427 S428 F429 K430 G431 S432 T433 W434 T435 L436 V437 D438 S439 A440 V441 Q442 N443 S444 K445 T446 Q447 Y448 V449 T450 R451 I452 I453 G454 I455 N456 M457 P458

- Molecule 7: Receptor binding protein

Chain X:



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K61 S62 Y63 G64 N65 I66 T67 A68 L69 R70 D71 I72 K73 E74 P75 G76 Y77 Y78 Y79 I80 G81 A82 R83 T84 L85 A86 T87 L88 L89 D90 R91 P92 D93 M94 E95 S96 L97 D98 V99 V100 L101 H102 V103 V104 P105 L106 D107 T108 S109 S110 K111 V112 V113 Q114 H115 L116 Y117 T118 L119 S120

T121 N122 N123 N124 Q125 I126 K127 M128 L129 Y130 R131 F132 V133 S134 G135 N136 S137 S138 S139 E140 W141 Q142 F143 I144 Q145 G146 L147 P148 S149 N150 K151 N152 A153 V154 I155 S156 G157 T158 N159 I160 L161 D162 I163 A164 S165 P166 G167 V168 Y169 F170 V171 M172 G173 M174 T175 G176 G177 M178 P179 S180

G181 V182 S183 S184 G185 F186 L187 D188 L189 S190 V191 D192 A193 N194 D195 N196 R197 L198 A199 R200 L201 T202 D203 A204 E205 T206 G207 K208 E209 Y210 T211 S212 I213 K214 K215 P216 T217 G218 T219 Y220 T221 A222 W223 K224 K225 E226 F227 E228 P229 K230 D231 M232 E233 K234 Y235 L236 L237 S238 S239 I240

R241 D242 D243 G244 S245 A246 S247 F248 P249 L250 L251 V252 Y253 T254 S255 D256 S257 K258 T259 F260 Q261 Q262 A263 I264 I265 D266 H267 I268 D269 R270 T271 G272 Q273 T274 T275 F276 T277 F278 Y279 V280 Q281 G282 G283 V284 S285 G286 S287 P288 M289 S290 N291 S292 C293 R294 G295 L296 F297 M298 S299 D300

T301 P302 N303 T304 S305 S306 L307 H308 G309 V310 Y311 N312 A313 I314 G315 T316 D317 G318 R319 N320 V321 T322 G323 S324 V325 V326 G327 S328 N329 W330 T331 S332 P333 K334 T335 S336 P337 S338 H339 K340 E341 L342 W343 T344 G345 A346 Q347 S348 F349 L350 S351 T352 G353 T354 T355 K356 N357 L358 S359 D360

D361 I362 S363 N364 Y365 S366 Y367 V368 E369 V370 Y371 T372 T373 H374 K375 T376 T377 E378 K379 T380 K381 G382 N383 D384 N385 T386 G387 T388 I389 C390 H391 K392 F393 Y394 L395 D396 G397 S398 G399 T400 Y401 V402 C403 S404 G405 T406 F407 V408 S409 G410 D411 R412 T413 D414 T415 K416 P417 P418 I419 T420

E421 F422 Y423 R424 V425 G426 V427 S428 F429 K430 G431 S432 T433 W434 T435 L436 V437 D438 S439 A440 V441 Q442 N443 S444 K445 T446 Q447 Y448 V449 T450 R451 I452 I453 G454 I455 N456 M457 P458

• Molecule 7: Receptor binding protein

Chain Y:

M1 A2 L3 N4 F5 T6 T7 I8 T9 E10 N11 N12 V13 I14 R15 D16 L17 T18 T19 Q20 V21 N22 N23 I24 G25 E26 E27 L28 T29 K30 E31 R32 N33 I34 F35 D36 I37 T38 D39 D40 L41 V42 Y43 N44 F45 N46 K47 S48 Q49 K50 I51 K52 L53 T54 D55 D56 K57 G58 L59 T60

K61 S62 Y63 G64 N65 I66 T67 A68 L69 R70 D71 I72 K73 E74 P75 G76 Y77 Y78 Y79 I80 G81 A82 R83 T84 L85 A86 T87 L88 L89 D90 R91 P92 D93 N94 E95 S96 L97 D98 V99 V100 L101 H102 V103 V104 P105 L106 D107 T108 S109 S110 K111 V112 V113 Q114 H115 L116 Y117 T118 L119 S120

T121 N122 N123 N124 Q125 I126 K127 M128 L129 Y130 R131 F132 V133 S134 G135 N136 S137 S138 S139 E140 W141 Q142 F143 I144 Q145 G146 L147 P148 S149 N150 K151 N152 A153 V154 I155 S156 G157 T158 N159 I160 L161 D162 I163 A164 S165 P166 G167 V168 Y169 F170 V171 M172 G173 M174 T175 G176 G177 M178 P179 S180

G181 V182 S183 S184 G185 F186 L187 D188 L189 S190 V191 D192 A193 N194 D195 N196 R197 L198 A199 R200 L201 T202 D203 A204 E205 T206 G207 K208 E209 Y210 T211 S212 I213 K214 K215 P216 T217 G218 T219 Y220 T221 A222 W223 K224 K225 E226 P227 E228 P229 K230 D231 M232 E233 K234 Y235 L236 L237 S238 S239 I240

R241 D242 D243 G244 S245 A246 S247 F248 P249 L250 L251 V252 Y253 T254 S255 D256 S257 K258 T259 F260 Q261 Q262 A263 I264 I265 D266 H267 I268 D269 R270 T271 G272 Q273 T274 T275 F276 T277 F278 Y279 V280 Q281 G282 G283 V284 S285 G286 S287 P288 M289 S290 N291 S292 C293 R294 G295 L296 F297 M298 S299 D300

T301 P302 N303 T304 S305 S306 L307 H308 G309 V310 Y311 N312 A313 I314 G315 T316 D317 G318 R319 N320 V321 T322 G323 S324 V325 V326 G327 S328 N329 W330 T331 S332 P333 K334 T335 S336 P337 S338 H339 K340 E341 L342 W343 T344 G345 A346 Q347 S348 F349 L350 S351 T352 G353 T354 T355 K356 N357 L358 S359 D360

D361 I362 S363 N364 Y365 S366 Y367 V368 E369 V370 Y371 T372 T373 H374 K375 T376 T377 E378 K379 T380 K381 G382 N383 D384 N385 T386 G387 T388 I389 C390 H391 K392 F393 Y394 L395 D396 G397 S398 G399 T400 Y401 V402 C403 S404 G405 T406 F407 V408 S409 G410 D411 R412 T413 D414 T415 K416 P417 P418 I419 T420

E421 F422 Y423 R424 V425 G426 V427 S428 F429 K430 G431 S432 T433 W434 T435 L436 V437 D438 S439 A440 V441 Q442 N443 S444 K445 T446 Q447 Y448 V449 T450 R451 I452 I453 G454 I455 N456 M457 P458

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	25203	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	761.04004, 761.04004, 761.04004	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	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	A	0.30	0/1902	0.56	0/2572
2	B	0.45	0/2803	0.68	0/3794
2	C	0.30	0/2795	0.56	0/3784
3	D	0.37	0/2281	0.64	0/3004
4	E	0.31	0/4280	0.57	0/5777
4	F	0.36	0/4392	0.63	2/5930 (0.0%)
4	G	0.37	0/4392	0.63	1/5930 (0.0%)
4	H	0.36	0/4392	0.63	3/5930 (0.1%)
4	I	0.34	0/4392	0.61	2/5930 (0.0%)
4	J	0.29	0/4392	0.56	0/5930
5	K	0.62	0/1407	0.91	1/1914 (0.1%)
5	L	0.64	0/1407	0.94	4/1914 (0.2%)
5	M	0.68	0/1407	0.97	4/1914 (0.2%)
5	N	0.68	0/1407	0.95	2/1914 (0.1%)
5	O	0.71	0/1407	0.98	3/1914 (0.2%)
5	P	0.69	0/1407	0.93	1/1914 (0.1%)
6	Q	0.33	0/7308	0.59	3/9911 (0.0%)
6	R	0.33	0/7308	0.58	1/9911 (0.0%)
6	S	0.45	0/7308	0.71	9/9911 (0.1%)
6	T	0.51	0/7308	0.78	15/9911 (0.2%)
6	U	0.48	0/7305	0.71	5/9905 (0.1%)
6	V	0.53	0/7308	0.79	13/9911 (0.1%)
7	W	0.45	0/1832	0.69	0/2287
7	X	0.45	0/1832	0.69	0/2287
7	Y	0.45	0/1832	0.69	0/2287
All	All	0.44	0/93804	0.69	69/126386 (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.

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Mol	Chain	#Chirality outliers	#Planarity outliers

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	1
4	H	0	1
5	O	0	1
6	S	0	2
6	T	0	2
6	V	0	2
All	All	0	9

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	1144	ARG	NE-CZ-NH2	10.01	125.30	120.30
6	T	477	ARG	NE-CZ-NH2	9.74	125.17	120.30
4	H	535	ARG	NE-CZ-NH2	9.35	124.98	120.30
5	M	65	ARG	NE-CZ-NH2	8.99	124.80	120.30
6	V	504	ARG	NE-CZ-NH2	8.80	124.70	120.30
6	T	286	ARG	NE-CZ-NH2	8.78	124.69	120.30
6	Q	1144	ARG	NE-CZ-NH2	8.20	124.40	120.30
6	U	477	ARG	NE-CZ-NH2	8.18	124.39	120.30
5	O	65	ARG	NE-CZ-NH2	7.89	124.25	120.30
6	T	272	ARG	NE-CZ-NH2	7.89	124.24	120.30
4	G	472	ARG	NE-CZ-NH2	7.86	124.23	120.30
6	V	477	ARG	NE-CZ-NH2	7.44	124.02	120.30
6	T	504	ARG	NE-CZ-NH2	7.19	123.89	120.30
6	R	1128	ARG	NE-CZ-NH2	7.18	123.89	120.30
4	H	86	ARG	NE-CZ-NH2	6.77	123.68	120.30
6	U	504	ARG	NE-CZ-NH2	6.76	123.68	120.30
6	V	286	ARG	NE-CZ-NH2	6.70	123.65	120.30
6	S	465	ARG	NE-CZ-NH2	6.62	123.61	120.30
6	S	271	ARG	NE-CZ-NH2	6.62	123.61	120.30
6	T	286	ARG	NE-CZ-NH1	-6.55	117.03	120.30
5	N	65	ARG	NE-CZ-NH2	6.50	123.55	120.30
6	T	406	ARG	NE-CZ-NH2	6.39	123.50	120.30
5	O	159	ARG	NE-CZ-NH2	6.37	123.48	120.30
6	V	234	ARG	NE-CZ-NH2	6.36	123.48	120.30
6	T	465	ARG	NE-CZ-NH2	6.36	123.48	120.30
6	V	295	PHE	CB-CG-CD1	-6.26	116.42	120.80
5	L	65	ARG	NE-CZ-NH2	6.14	123.37	120.30
6	V	1150	ARG	NE-CZ-NH2	6.10	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	272	ARG	NE-CZ-NH2	6.02	123.31	120.30
6	V	271	ARG	NE-CZ-NH2	5.96	123.28	120.30
5	O	118	ARG	NE-CZ-NH2	5.89	123.25	120.30
6	U	465	ARG	NE-CZ-NH2	5.88	123.24	120.30
6	S	286	ARG	NE-CZ-NH2	5.86	123.23	120.30
5	L	159	ARG	NE-CZ-NH2	5.84	123.22	120.30
5	M	118	ARG	NE-CZ-NH2	5.83	123.21	120.30
6	V	88	ARG	NE-CZ-NH2	5.78	123.19	120.30
4	F	64	ARG	NE-CZ-NH2	5.75	123.18	120.30
5	M	168	ARG	NE-CZ-NH2	5.75	123.18	120.30
6	Q	1026	ARG	NE-CZ-NH2	5.74	123.17	120.30
5	P	65	ARG	NE-CZ-NH2	5.69	123.14	120.30
5	L	118	ARG	NE-CZ-NH2	5.67	123.14	120.30
6	V	358	ARG	NE-CZ-NH2	5.66	123.13	120.30
6	T	272	ARG	NE-CZ-NH1	-5.62	117.49	120.30
6	T	1109	ARG	NE-CZ-NH2	5.62	123.11	120.30
5	N	118	ARG	NE-CZ-NH2	5.60	123.10	120.30
6	T	271	ARG	NE-CZ-NH2	5.59	123.10	120.30
6	T	1066	ARG	NE-CZ-NH2	5.58	123.09	120.30
6	V	1109	ARG	NE-CZ-NH2	5.56	123.08	120.30
6	V	283	ARG	NE-CZ-NH2	5.52	123.06	120.30
6	V	272	ARG	NE-CZ-NH2	5.48	123.04	120.30
6	T	1144	ARG	NE-CZ-NH1	-5.48	117.56	120.30
6	V	406	ARG	NE-CZ-NH2	5.41	123.00	120.30
6	T	358	ARG	NE-CZ-NH2	5.39	123.00	120.30
6	T	465	ARG	CD-NE-CZ	5.38	131.13	123.60
4	I	380	ARG	NE-CZ-NH2	5.36	122.98	120.30
6	S	406	ARG	NE-CZ-NH2	5.34	122.97	120.30
6	S	271	ARG	NE-CZ-NH1	-5.32	117.64	120.30
6	S	286	ARG	NE-CZ-NH1	-5.23	117.68	120.30
4	F	380	ARG	NE-CZ-NH2	5.21	122.91	120.30
6	U	1150	ARG	NE-CZ-NH2	5.21	122.90	120.30
4	I	388	ARG	NE-CZ-NH2	5.18	122.89	120.30
5	K	118	ARG	NE-CZ-NH2	5.16	122.88	120.30
4	H	380	ARG	NE-CZ-NH2	5.15	122.88	120.30
6	U	272	ARG	NE-CZ-NH2	5.11	122.86	120.30
6	S	465	ARG	CD-NE-CZ	5.06	130.68	123.60
6	Q	1143	ARG	NE-CZ-NH2	5.04	122.82	120.30
5	M	65	ARG	NE-CZ-NH1	-5.04	117.78	120.30
6	S	234	ARG	NE-CZ-NH2	5.03	122.82	120.30
5	L	168	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	363	ARG	Sidechain
4	H	535	ARG	Sidechain
5	O	158	ASN	Peptide
6	S	272	ARG	Sidechain
6	S	286	ARG	Sidechain
6	T	286	ARG	Sidechain
6	T	327	ARG	Sidechain
6	V	286	ARG	Sidechain
6	V	295	PHE	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	A	1871	0	1828	9	0
2	B	2760	0	2729	7	0
2	C	2752	0	2717	8	0
3	D	2252	0	1652	12	0
4	E	4213	0	4167	20	0
4	F	4321	0	4280	17	0
4	G	4321	0	4280	15	0
4	H	4321	0	4280	11	0
4	I	4321	0	4280	22	0
4	J	4321	0	4280	14	0
5	K	1378	0	1361	7	0
5	L	1378	0	1361	0	0
5	M	1378	0	1361	0	0
5	N	1378	0	1361	1	0
5	O	1378	0	1361	1	0
5	P	1378	0	1361	0	0
6	Q	7166	0	6971	14	0
6	R	7166	0	6971	17	0
6	S	7166	0	6971	6	0
6	T	7166	0	6971	10	0
6	U	7165	0	6969	7	0
6	V	7166	0	6971	20	0
7	W	1833	0	520	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	1833	0	520	0	0
7	Y	1833	0	520	0	0
All	All	92215	0	86043	183	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 (183) 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)
6:V:295:PHE:CE2	7:W:96:SER:N	1.85	1.39
6:V:344:SER:CB	7:W:162:ASP:CA	2.31	1.09
6:V:295:PHE:CD2	7:W:96:SER:N	2.13	1.06
6:V:344:SER:OG	7:W:162:ASP:CA	2.11	0.98
6:V:295:PHE:CD2	7:W:96:SER:CA	2.50	0.94
3:D:177:ASP:OD1	5:K:168:ARG:NH1	2.02	0.91
6:V:344:SER:HB3	7:W:162:ASP:CA	2.00	0.90
3:D:177:ASP:CG	5:K:168:ARG:HH11	1.74	0.89
6:V:295:PHE:HE2	7:W:96:SER:H	0.90	0.84
6:U:1077:THR:CA	6:U:1078:LYS:N	2.41	0.83
6:V:344:SER:HB3	7:W:162:ASP:C	2.00	0.81
6:V:344:SER:HB3	7:W:162:ASP:O	1.83	0.79
6:V:295:PHE:CE2	7:W:96:SER:CA	2.68	0.76
3:D:33:ASN:OD1	3:D:37:ASN:ND2	2.20	0.74
2:B:191:ARG:NH1	2:C:187:GLU:OE1	2.21	0.74
3:D:179:ALA:HB1	5:K:80:TYR:HA	1.71	0.71
6:U:1077:THR:O	6:U:1078:LYS:N	2.26	0.69
3:D:338:GLN:O	6:T:4:ASN:HB3	1.93	0.69
6:U:1077:THR:CA	6:U:1077:THR:O	2.41	0.68
2:C:85:PHE:O	2:C:158:ARG:NH2	2.26	0.68
4:G:557:ASN:OD1	4:H:569:ARG:NH2	2.25	0.68
6:U:83:ILE:O	6:U:88:ARG:NH2	2.26	0.68
6:S:83:ILE:O	6:S:88:ARG:NH2	2.26	0.68
6:Q:83:ILE:O	6:Q:88:ARG:NH2	2.27	0.67
4:F:536:LYS:NZ	4:F:541:GLU:OE1	2.26	0.67
4:F:371:ASN:OD1	4:F:442:GLN:NE2	2.29	0.65
4:E:557:ASN:OD1	4:F:569:ARG:NH2	2.31	0.64
4:I:141:ASP:OD1	4:I:141:ASP:N	2.27	0.64
6:Q:88:ARG:NH1	6:Q:143:GLU:OE1	2.31	0.64
6:Q:504:ARG:NH1	6:S:480:ASN:OD1	2.32	0.63
6:Q:480:ASN:OD1	6:R:504:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:371:ASN:OD1	4:H:442:GLN:NE2	2.33	0.62
3:D:177:ASP:CG	5:K:168:ARG:NH1	2.51	0.62
4:I:124:GLU:N	4:I:124:GLU:OE1	2.33	0.61
6:V:295:PHE:HE2	7:W:96:SER:N	1.53	0.60
4:J:329:HIS:ND1	4:J:360:GLU:OE2	2.35	0.60
4:I:516:ARG:NH1	4:J:428:GLU:OE2	2.35	0.59
4:J:129:SER:O	4:J:152:ASN:ND2	2.36	0.59
2:C:57:TRP:NE1	2:C:61:GLU:OE1	2.35	0.59
4:H:74:LEU:O	4:H:78:SER:N	2.36	0.58
4:E:386:ASN:O	4:E:479:THR:OG1	2.22	0.58
4:E:70:ASP:OD1	4:E:404:ARG:NH1	2.36	0.58
1:A:80:ASN:ND2	4:E:83:THR:OG1	2.37	0.57
6:V:344:SER:CB	7:W:162:ASP:O	2.52	0.57
2:B:12:LYS:NZ	3:D:34:GLU:OE2	2.36	0.57
6:R:480:ASN:OD1	6:S:504:ARG:NH1	2.37	0.57
4:J:4:GLU:OE2	4:J:8:ARG:NH2	2.38	0.57
3:D:338:GLN:O	6:T:4:ASN:CB	2.53	0.57
4:J:94:ASP:OD1	4:J:323:LYS:NZ	2.38	0.56
6:V:344:SER:HG	7:W:162:ASP:CA	2.18	0.55
4:J:158:TYR:OH	4:J:162:GLU:N	2.38	0.55
1:A:131:ILE:HG21	4:E:22:THR:HG23	1.89	0.55
3:D:179:ALA:CB	5:K:80:TYR:HA	2.37	0.54
4:F:482:ASP:N	4:F:482:ASP:OD1	2.39	0.54
4:G:151:GLY:O	4:G:226:LYS:NZ	2.36	0.54
4:F:172:ASP:O	4:F:176:GLN:N	2.40	0.54
4:J:153:ILE:HG23	4:J:154:PHE:HD1	1.74	0.53
6:R:216:ASP:OD1	6:R:217:ALA:N	2.41	0.53
4:G:371:ASN:OD1	4:G:442:GLN:NE2	2.41	0.53
4:I:535:ARG:NH1	4:I:539:ASP:OD2	2.41	0.53
4:I:229:GLU:N	4:I:229:GLU:OE1	2.41	0.53
4:H:153:ILE:HG23	4:H:154:PHE:HD1	1.72	0.53
4:E:172:ASP:O	4:E:176:GLN:N	2.40	0.53
4:E:148:ASP:OD1	4:E:149:ASN:N	2.41	0.52
4:G:148:ASP:OD1	4:G:149:ASN:N	2.42	0.52
4:H:557:ASN:OD1	4:I:569:ARG:NH2	2.42	0.52
4:H:153:ILE:HG22	4:H:248:VAL:O	2.09	0.52
4:E:164:ASN:OD1	4:E:165:ALA:N	2.42	0.52
4:E:517:THR:N	4:F:569:ARG:O	2.41	0.52
4:E:34:LYS:NZ	4:E:495:GLU:OE2	2.31	0.51
4:E:206:ILE:HG22	4:E:210:ILE:CD1	2.39	0.51
4:E:153:ILE:HG23	4:E:154:PHE:CD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:167:PHE:HD1	4:G:241:ILE:HD11	1.75	0.51
4:E:464:ARG:O	4:E:466:ARG:NH2	2.43	0.51
6:Q:477:ARG:NH1	6:R:479:ASP:OD1	2.40	0.50
2:B:232:ASP:OD1	2:B:233:THR:N	2.44	0.50
6:R:239:LYS:NZ	6:R:454:ASP:OD1	2.36	0.50
6:R:818:ASP:OD1	6:R:820:GLN:N	2.43	0.50
4:H:172:ASP:O	4:H:176:GLN:N	2.42	0.50
6:Q:426:ASN:OD1	6:Q:427:ILE:N	2.45	0.50
4:I:513:ILE:HG23	4:J:572:LYS:HA	1.92	0.50
1:A:30:ASP:N	1:A:30:ASP:OD1	2.45	0.49
4:F:123:LEU:HD12	4:F:303:PHE:CE2	2.47	0.49
1:A:124:ASP:OD1	1:A:125:LEU:N	2.46	0.49
2:B:16:LYS:NZ	3:D:30:ASP:OD2	2.45	0.49
1:A:131:ILE:HG21	4:E:22:THR:CG2	2.44	0.48
2:B:191:ARG:O	2:B:196:SER:OG	2.30	0.48
6:V:810:GLY:N	6:V:937:GLY:O	2.45	0.48
4:E:509:GLU:HA	4:E:513:ILE:HD12	1.95	0.48
4:F:148:ASP:OD1	4:F:149:ASN:N	2.46	0.48
4:F:124:GLU:O	4:F:133:ARG:N	2.46	0.48
6:Q:479:ASP:OD1	6:S:477:ARG:NH1	2.45	0.48
4:E:206:ILE:HG22	4:E:210:ILE:HD11	1.95	0.48
4:H:114:ASN:N	4:H:313:ASN:OD1	2.47	0.48
4:I:557:ASN:N	4:I:557:ASN:OD1	2.47	0.48
4:I:123:LEU:HD12	4:I:303:PHE:CE2	2.49	0.47
3:D:177:ASP:OD2	5:K:168:ARG:NH1	2.48	0.47
4:I:517:THR:N	4:J:569:ARG:O	2.45	0.47
4:G:167:PHE:CB	4:G:183:LEU:HD23	2.45	0.47
4:I:40:GLY:HA3	4:I:338:LEU:HD12	1.97	0.47
1:A:54:GLU:OE1	1:A:54:GLU:N	2.42	0.46
6:T:818:ASP:OD1	6:T:820:GLN:N	2.43	0.46
4:I:435:LEU:HD22	4:I:460:ILE:HD13	1.96	0.46
4:I:475:ASP:OD1	4:I:476:ASP:N	2.45	0.46
1:A:142:LEU:O	1:A:157:SER:OG	2.31	0.46
4:G:211:ASN:ND2	4:G:218:ALA:O	2.48	0.46
4:I:312:THR:HG22	4:I:314:GLY:H	1.81	0.46
4:I:482:ASP:OD1	4:I:482:ASP:N	2.49	0.46
6:R:20:ARG:NH1	6:S:120:ASP:OD2	2.44	0.46
6:R:88:ARG:NH1	6:R:143:GLU:OE1	2.49	0.46
4:E:516:ARG:NH1	4:F:426:ILE:O	2.49	0.46
2:C:225:ASP:OD1	2:C:229:ASN:N	2.49	0.46
4:I:172:ASP:O	4:I:176:GLN:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:153:ILE:HG23	4:H:154:PHE:CD1	2.50	0.45
4:G:126:ASN:ND2	4:G:129:SER:OG	2.46	0.45
6:T:20:ARG:NH1	6:U:120:ASP:OD2	2.44	0.45
4:F:375:GLU:OE1	4:F:375:GLU:N	2.47	0.45
2:C:324:ASP:OD1	2:C:325:ASN:N	2.49	0.45
6:Q:1084:SER:OG	6:Q:1086:ASP:OD1	2.34	0.45
4:G:40:GLY:HA3	4:G:338:LEU:HD12	1.99	0.45
4:G:167:PHE:CD1	4:G:241:ILE:HD11	2.52	0.45
3:D:179:ALA:HB1	5:K:81:GLY:H	1.82	0.45
6:Q:810:GLY:N	6:Q:937:GLY:O	2.45	0.44
4:E:74:LEU:O	4:E:78:SER:N	2.50	0.44
4:G:180:ARG:NE	4:G:194:ASP:OD1	2.42	0.44
4:J:114:ASN:OD1	4:J:313:ASN:N	2.49	0.44
4:I:153:ILE:HG22	4:I:248:VAL:O	2.18	0.44
6:Q:239:LYS:NZ	6:Q:454:ASP:OD1	2.42	0.44
4:I:114:ASN:OD1	4:I:313:ASN:N	2.51	0.44
4:I:312:THR:HG22	4:I:314:GLY:N	2.32	0.44
4:J:183:LEU:O	4:J:190:VAL:N	2.48	0.44
6:R:92:ASN:ND2	6:R:145:MET:O	2.51	0.44
6:R:426:ASN:OD1	6:R:427:ILE:N	2.49	0.44
4:I:134:LEU:N	4:I:147:TYR:O	2.51	0.43
4:H:79:ASN:ND2	4:H:419:GLY:O	2.50	0.43
6:R:518:ASP:OD1	6:T:347:THR:HB	2.18	0.43
6:T:92:ASN:ND2	6:T:145:MET:O	2.51	0.43
6:Q:50:LEU:HA	6:R:87:ILE:HD12	2.01	0.43
1:A:214:VAL:HG12	1:A:218:ILE:HD12	2.00	0.43
4:I:137:ILE:HD12	4:I:305:LEU:HD21	2.01	0.43
6:T:122:SER:O	6:V:13:ARG:NH2	2.51	0.43
4:F:153:ILE:HG22	4:F:248:VAL:O	2.19	0.43
6:V:884:GLU:OE1	6:V:884:GLU:N	2.48	0.43
4:G:52:GLU:OE2	4:G:54:ARG:NE	2.51	0.42
6:Q:13:ARG:NH2	6:R:122:SER:O	2.51	0.42
4:E:210:ILE:HG21	4:E:218:ALA:HB2	2.00	0.42
6:T:568:GLU:OE1	6:T:862:ARG:NH1	2.52	0.42
4:E:185:VAL:HG23	4:E:190:VAL:CG2	2.48	0.42
6:R:568:GLU:OE1	6:R:862:ARG:NH1	2.52	0.42
1:A:48:GLU:N	1:A:48:GLU:OE1	2.52	0.42
4:F:544:ASP:OD1	4:F:545:PHE:N	2.52	0.42
4:G:38:LEU:HD21	4:G:415:VAL:HG13	2.01	0.42
6:Q:531:GLU:OE1	6:Q:531:GLU:N	2.46	0.42
2:C:253:ASP:OD1	2:C:254:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:1104:ASN:OD1	6:V:1107:PHE:N	2.51	0.42
4:F:34:LYS:NZ	4:F:495:GLU:OE2	2.36	0.42
5:N:6:TYR:CE2	5:N:99:LYS:HE2	2.54	0.42
6:U:810:GLY:N	6:U:937:GLY:O	2.52	0.42
6:V:531:GLU:OE1	6:V:531:GLU:N	2.46	0.42
4:I:167:PHE:HB3	4:I:241:ILE:HD11	2.02	0.42
4:J:505:LYS:NZ	4:J:509:GLU:OE2	2.52	0.42
6:Q:884:GLU:OE1	6:Q:884:GLU:N	2.48	0.42
4:F:153:ILE:HG23	4:F:154:PHE:CD1	2.54	0.42
4:H:244:LYS:O	4:H:246:VAL:HG23	2.20	0.42
5:O:134:LYS:HB3	6:V:8:SER:OG	2.18	0.42
6:V:295:PHE:CD2	6:V:295:PHE:N	2.87	0.42
4:G:172:ASP:O	4:G:176:GLN:N	2.52	0.41
6:T:94:ASP:OD1	6:T:95:SER:N	2.53	0.41
6:R:94:ASP:OD1	6:R:95:SER:N	2.53	0.41
2:C:281:GLN:NE2	2:C:345:VAL:O	2.51	0.41
4:F:411:TYR:O	4:F:415:VAL:HG23	2.21	0.41
6:R:892:VAL:HG12	6:R:934:LEU:HD23	2.03	0.41
6:T:892:VAL:HG12	6:T:934:LEU:HD23	2.02	0.41
2:B:268:VAL:HG23	2:B:321:VAL:HG22	2.01	0.41
6:S:65:GLY:O	6:S:77:ASN:ND2	2.54	0.41
2:C:257:VAL:O	2:C:259:LYS:N	2.54	0.41
4:F:188:GLN:N	4:F:188:GLN:OE1	2.54	0.41
6:U:65:GLY:O	6:U:77:ASN:ND2	2.54	0.41
4:J:173:GLU:O	4:J:176:GLN:NE2	2.54	0.40
4:J:437:VAL:HG11	4:J:440:LEU:HD21	2.04	0.40
2:B:2:LYS:O	2:B:3:THR:OG1	2.32	0.40
4:G:167:PHE:HB2	4:G:183:LEU:HD23	2.03	0.40
6:R:810:GLY:N	6:R:937:GLY:O	2.50	0.40

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	A	232/234 (99%)	223 (96%)	9 (4%)	0	100	100
2	B	346/348 (99%)	341 (99%)	5 (1%)	0	100	100
2	C	345/348 (99%)	339 (98%)	6 (2%)	0	100	100
3	D	367/1019 (36%)	354 (96%)	13 (4%)	0	100	100
4	E	534/587 (91%)	502 (94%)	31 (6%)	1 (0%)	44	78
4	F	547/587 (93%)	516 (94%)	31 (6%)	0	100	100
4	G	547/587 (93%)	521 (95%)	26 (5%)	0	100	100
4	H	547/587 (93%)	524 (96%)	23 (4%)	0	100	100
4	I	547/587 (93%)	526 (96%)	21 (4%)	0	100	100
4	J	547/587 (93%)	522 (95%)	25 (5%)	0	100	100
5	K	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
5	L	174/194 (90%)	170 (98%)	4 (2%)	0	100	100
5	M	174/194 (90%)	165 (95%)	9 (5%)	0	100	100
5	N	174/194 (90%)	169 (97%)	5 (3%)	0	100	100
5	O	174/194 (90%)	169 (97%)	5 (3%)	0	100	100
5	P	174/194 (90%)	170 (98%)	4 (2%)	0	100	100
6	Q	900/1152 (78%)	876 (97%)	24 (3%)	0	100	100
6	R	900/1152 (78%)	872 (97%)	27 (3%)	1 (0%)	48	83
6	S	900/1152 (78%)	872 (97%)	28 (3%)	0	100	100
6	T	900/1152 (78%)	869 (97%)	30 (3%)	1 (0%)	48	83
6	U	898/1152 (78%)	866 (96%)	32 (4%)	0	100	100
6	V	900/1152 (78%)	862 (96%)	35 (4%)	3 (0%)	37	72
7	W	456/458 (100%)	441 (97%)	15 (3%)	0	100	100
7	X	456/458 (100%)	446 (98%)	10 (2%)	0	100	100
7	Y	456/458 (100%)	445 (98%)	11 (2%)	0	100	100
All	All	12369/14921 (83%)	11926 (96%)	437 (4%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	V	325	ASP
6	T	57	ASP
6	R	519	ILE
6	V	346	GLY

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Mol	Chain	Res	Type
4	E	409	PRO
6	V	58	GLY

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	A	209/209 (100%)	208 (100%)	1 (0%)	86 90
2	B	311/311 (100%)	309 (99%)	2 (1%)	84 88
2	C	310/311 (100%)	310 (100%)	0	100 100
3	D	162/928 (18%)	162 (100%)	0	100 100
4	E	459/495 (93%)	456 (99%)	3 (1%)	81 87
4	F	471/495 (95%)	465 (99%)	6 (1%)	65 77
4	G	471/495 (95%)	467 (99%)	4 (1%)	79 85
4	H	471/495 (95%)	469 (100%)	2 (0%)	89 91
4	I	471/495 (95%)	464 (98%)	7 (2%)	60 75
4	J	471/495 (95%)	468 (99%)	3 (1%)	84 88
5	K	156/171 (91%)	154 (99%)	2 (1%)	65 77
5	L	156/171 (91%)	154 (99%)	2 (1%)	65 77
5	M	156/171 (91%)	152 (97%)	4 (3%)	41 61
5	N	156/171 (91%)	154 (99%)	2 (1%)	65 77
5	O	156/171 (91%)	155 (99%)	1 (1%)	84 88
5	P	156/171 (91%)	154 (99%)	2 (1%)	65 77
6	Q	800/1010 (79%)	797 (100%)	3 (0%)	89 91
6	R	800/1010 (79%)	799 (100%)	1 (0%)	92 95
6	S	800/1010 (79%)	798 (100%)	2 (0%)	91 92
6	T	800/1010 (79%)	798 (100%)	2 (0%)	91 92
6	U	800/1010 (79%)	798 (100%)	2 (0%)	91 92
6	V	800/1010 (79%)	795 (99%)	5 (1%)	84 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9542/11815 (81%)	9486 (99%)	56 (1%)	82 88

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
2	B	90	ASP
2	B	271	SER
4	E	269	GLN
4	E	354	GLU
4	E	428	GLU
4	F	114	ASN
4	F	247	TYR
4	F	453	ASN
4	F	481	ASN
4	F	482	ASP
4	F	516	ARG
4	G	13	ARG
4	G	225	ASP
4	G	339	SER
4	G	436	ARG
4	H	436	ARG
4	H	453	ASN
4	I	138	PHE
4	I	141	ASP
4	I	167	PHE
4	I	241	ILE
4	I	247	TYR
4	I	436	ARG
4	I	557	ASN
4	J	54	ARG
4	J	202	TYR
4	J	252	PHE
5	K	172	GLU
5	K	176	ASN
5	L	156	PHE
5	L	176	ASN
5	M	99	LYS
5	M	157	GLN
5	M	168	ARG
5	M	176	ASN
5	N	156	PHE

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Mol	Chain	Res	Type
5	N	176	ASN
5	O	176	ASN
5	P	38	ASN
5	P	176	ASN
6	Q	33	GLN
6	Q	574	GLN
6	Q	1134	GLU
6	R	574	GLN
6	S	33	GLN
6	S	574	GLN
6	T	57	ASP
6	T	574	GLN
6	U	33	GLN
6	U	574	GLN
6	V	33	GLN
6	V	60	LYS
6	V	358	ARG
6	V	574	GLN
6	V	1134	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	106	ASN
2	C	325	ASN
4	E	530	GLN
4	F	442	GLN
4	G	126	ASN
4	H	507	GLN
5	L	45	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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

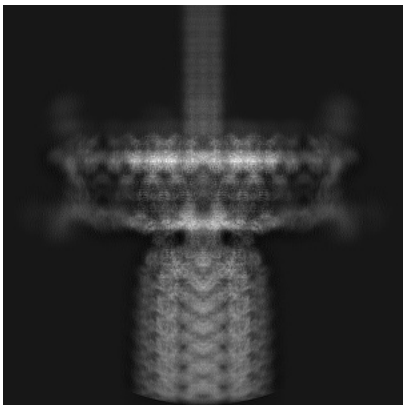
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19971. These allow visual inspection of the internal detail of the map and identification of artifacts.

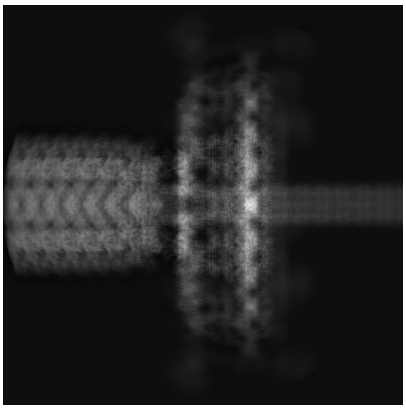
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

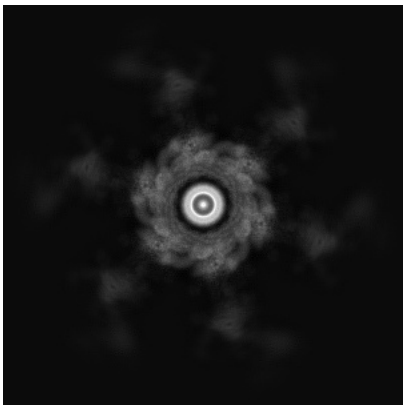
6.1.1 Primary map



X

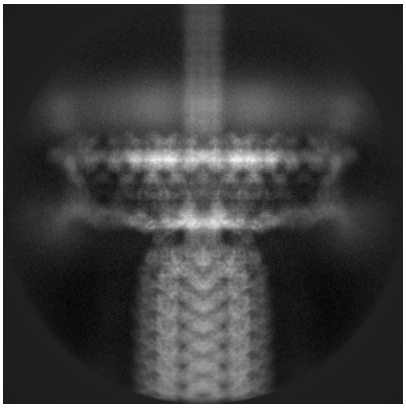


Y

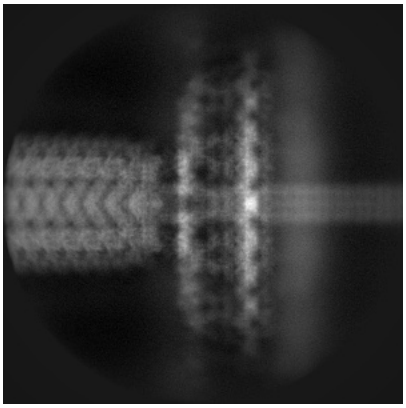


Z

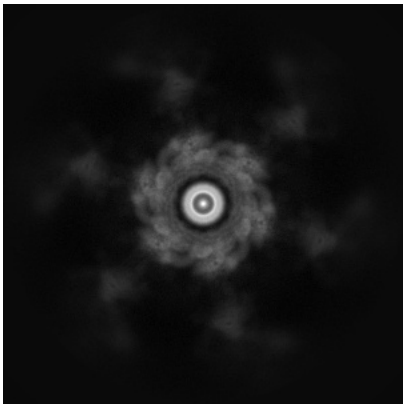
6.1.2 Raw map



X



Y

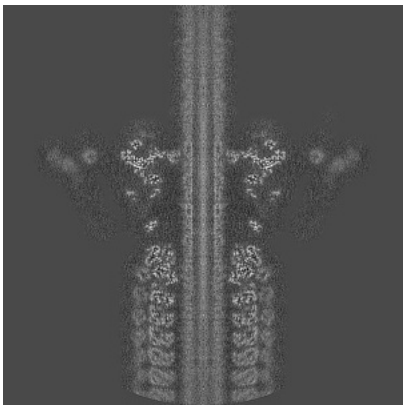


Z

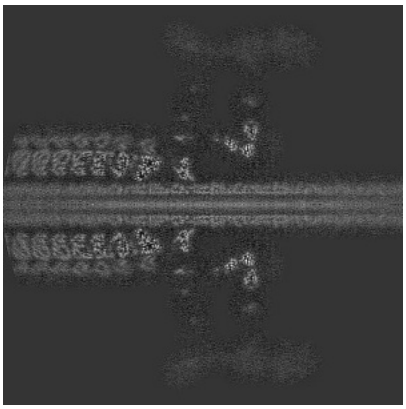
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

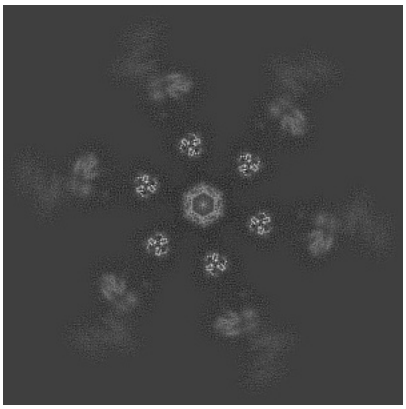
6.2.1 Primary map



X Index: 360

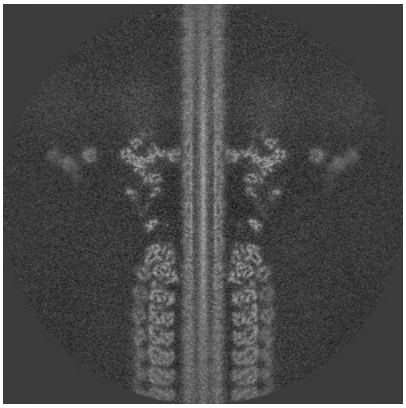


Y Index: 360

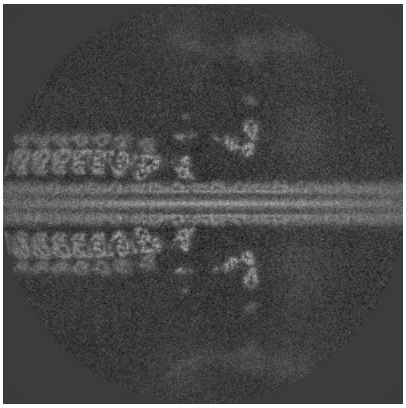


Z Index: 360

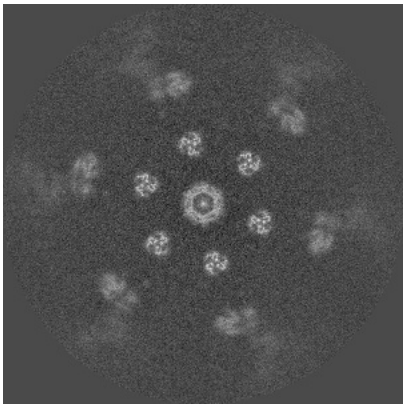
6.2.2 Raw map



X Index: 360



Y Index: 360

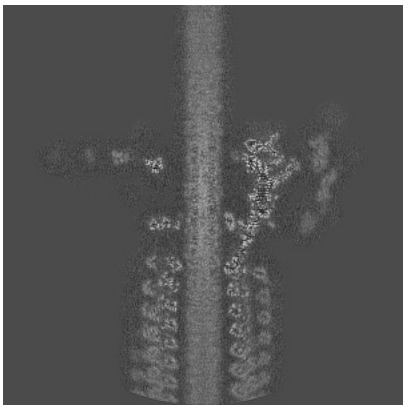


Z Index: 360

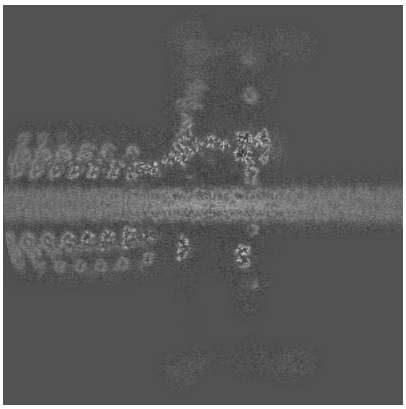
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

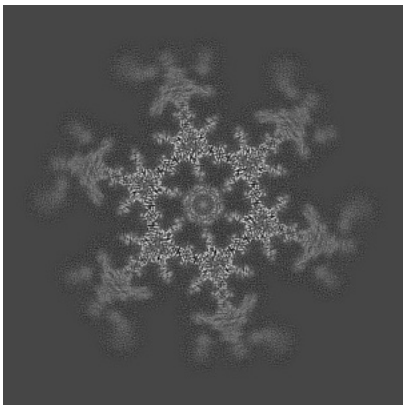
6.3.1 Primary map



X Index: 339

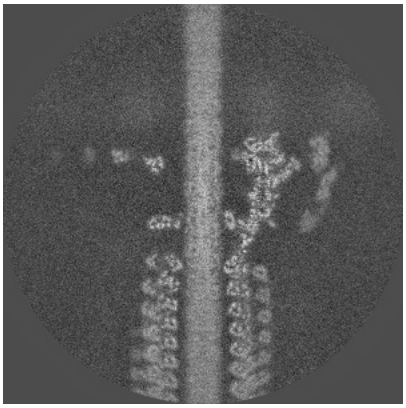


Y Index: 339

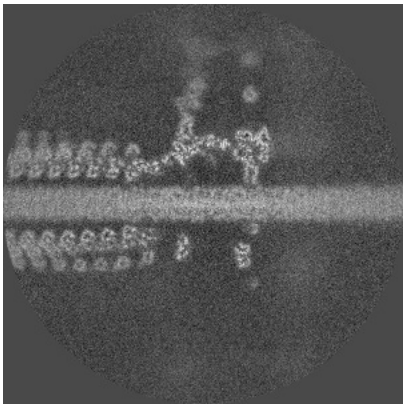


Z Index: 438

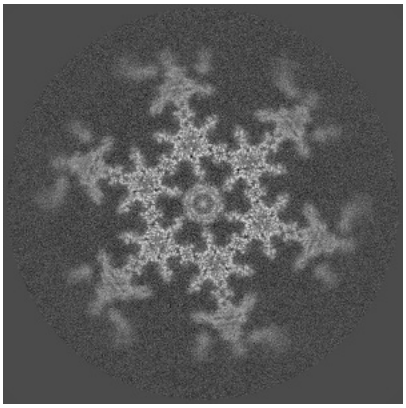
6.3.2 Raw map



X Index: 339



Y Index: 338

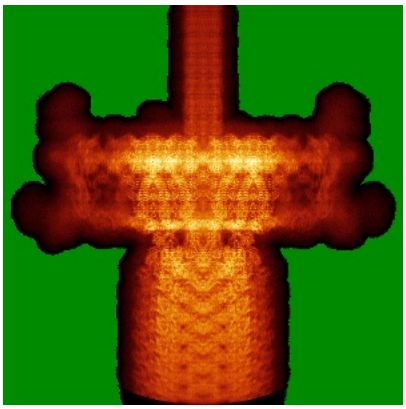


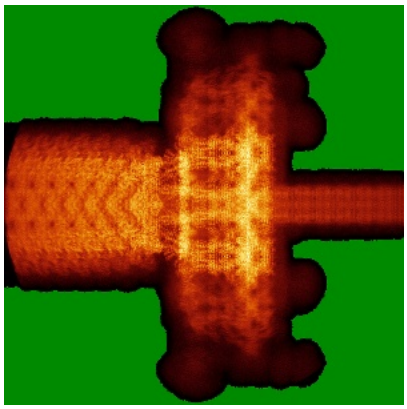
Z Index: 438

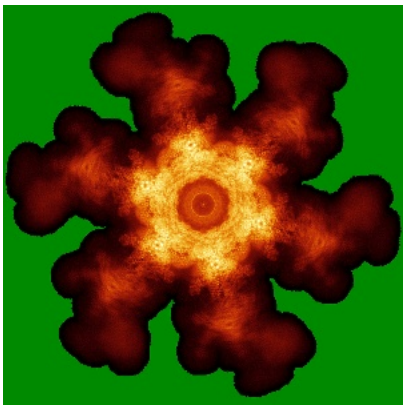
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

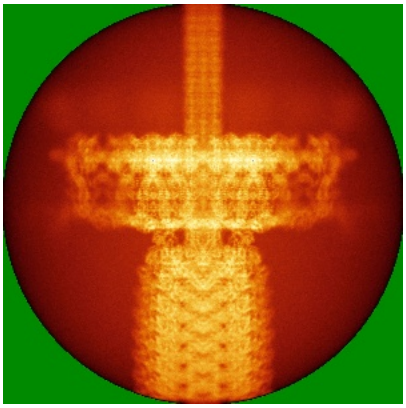
6.4.1 Primary map

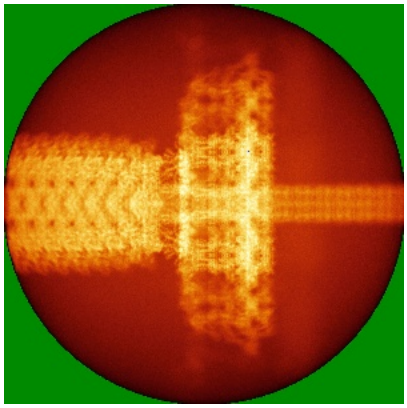

X

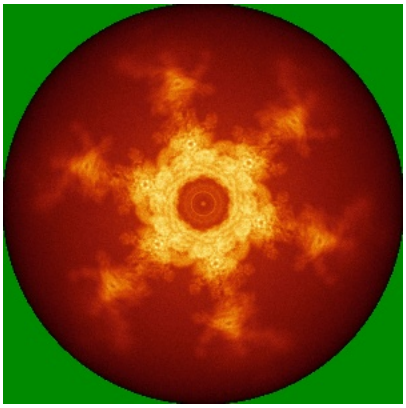

Y


Z

6.4.2 Raw map


X

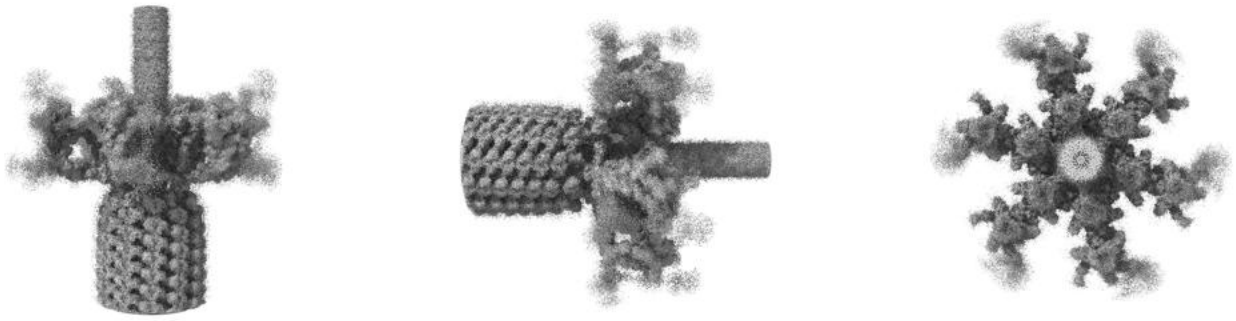

Y


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)

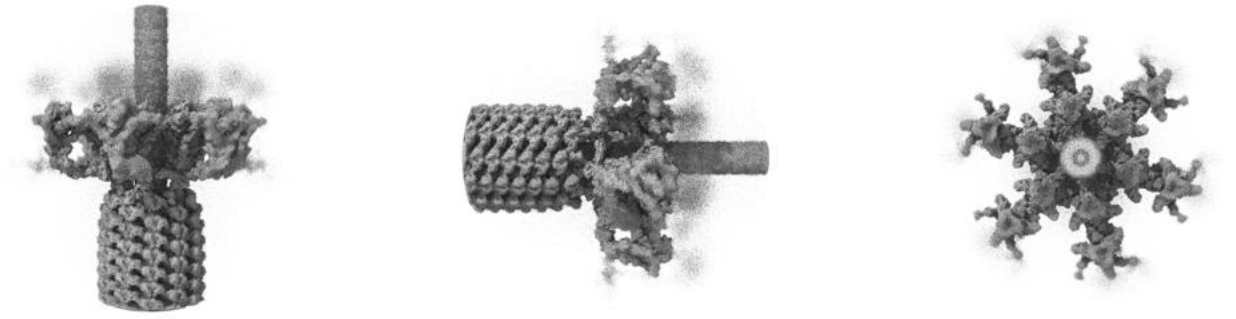
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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.

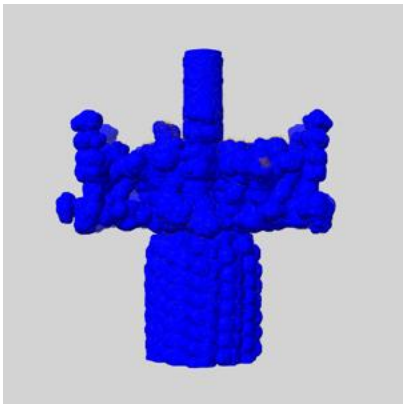
6.6 Mask visualisation (i)

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

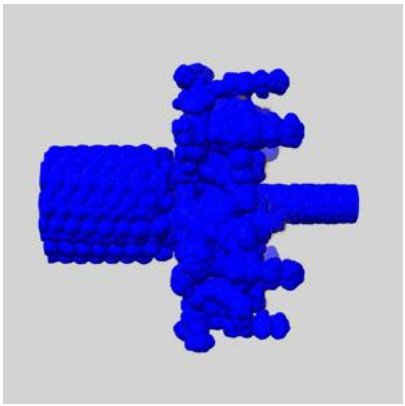
A mask typically either:

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

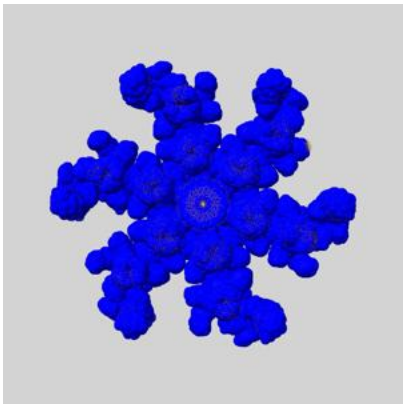
6.6.1 emd_19971_msk_1.map (i)



X



Y

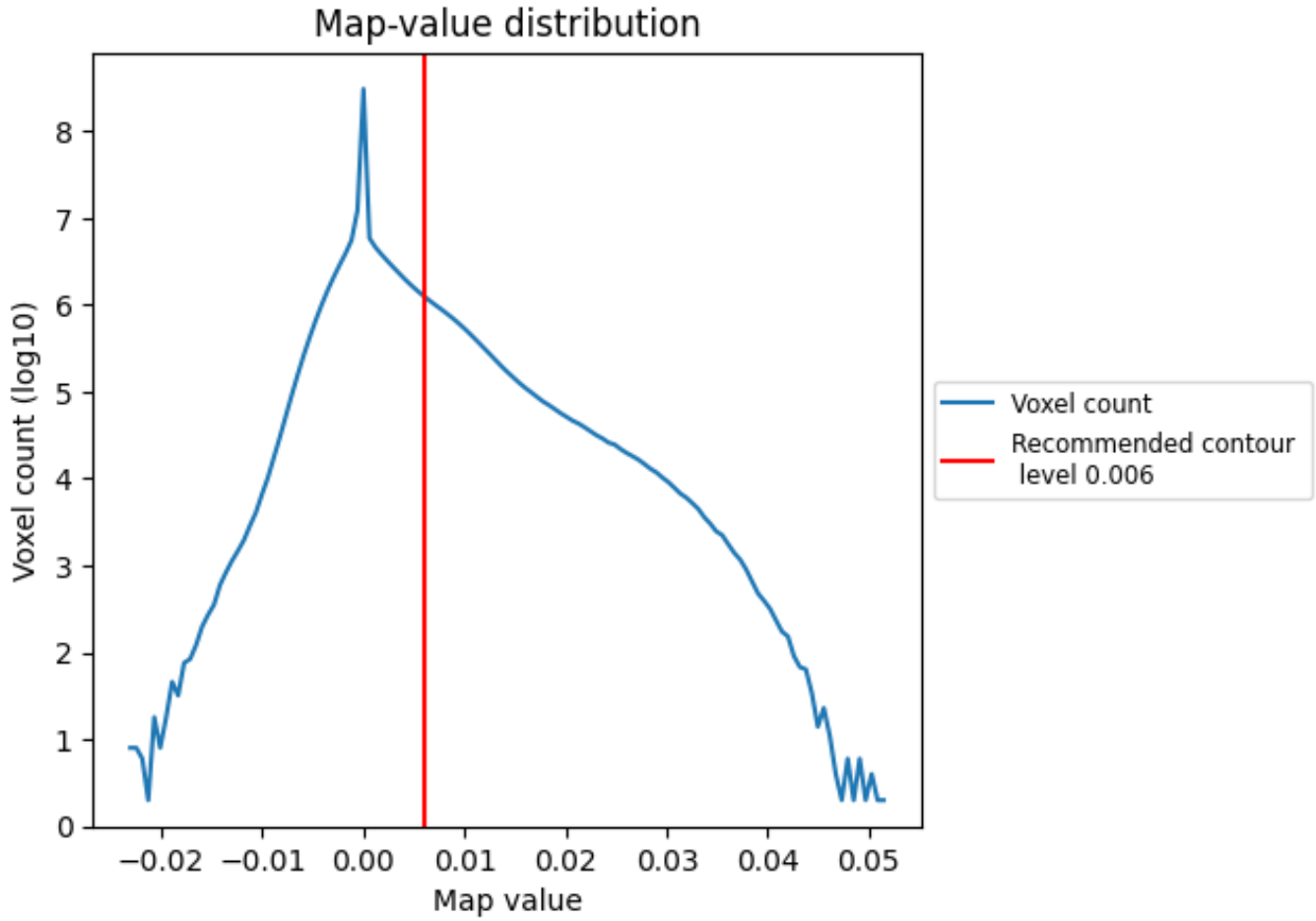


Z

7 Map analysis

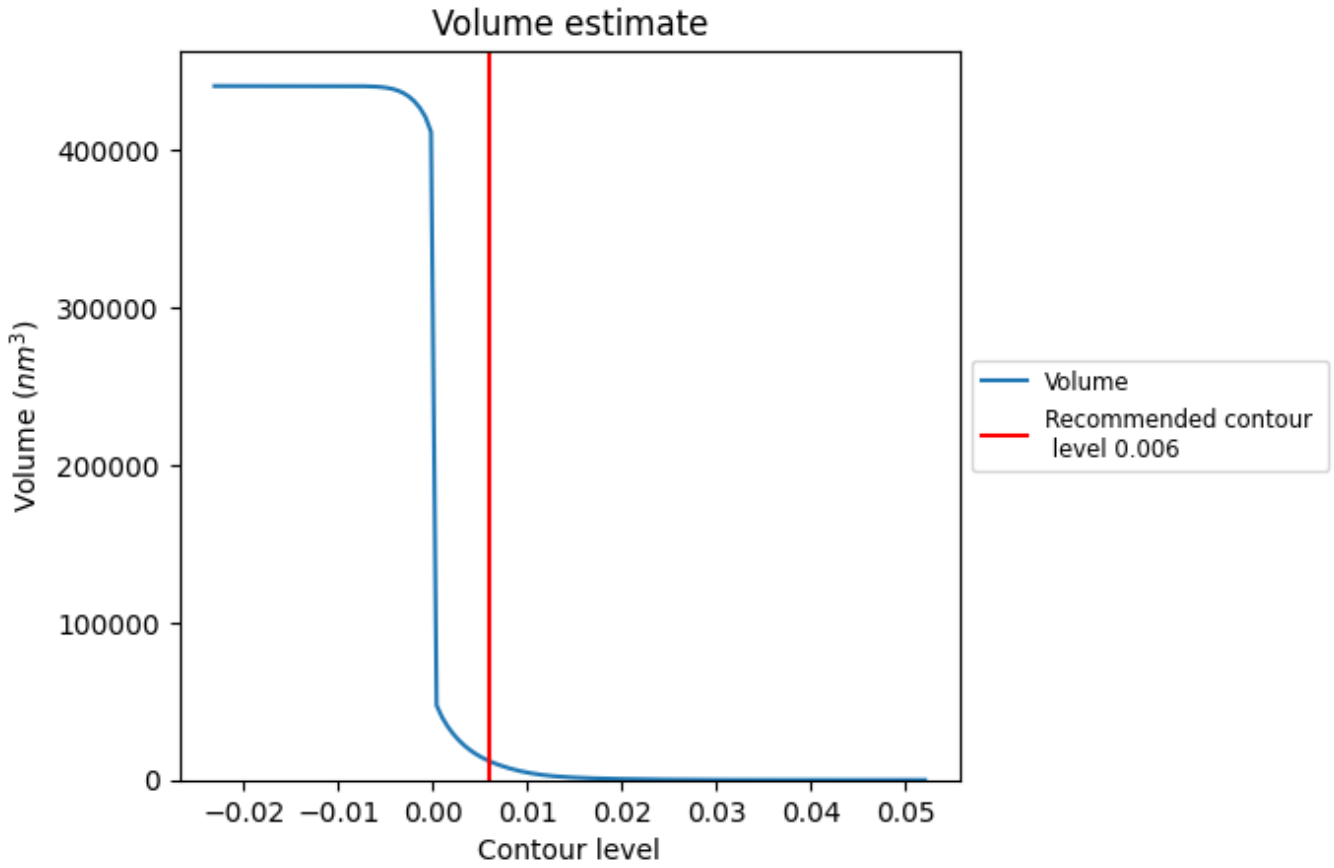
This section contains the results of statistical analysis of the map.

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.

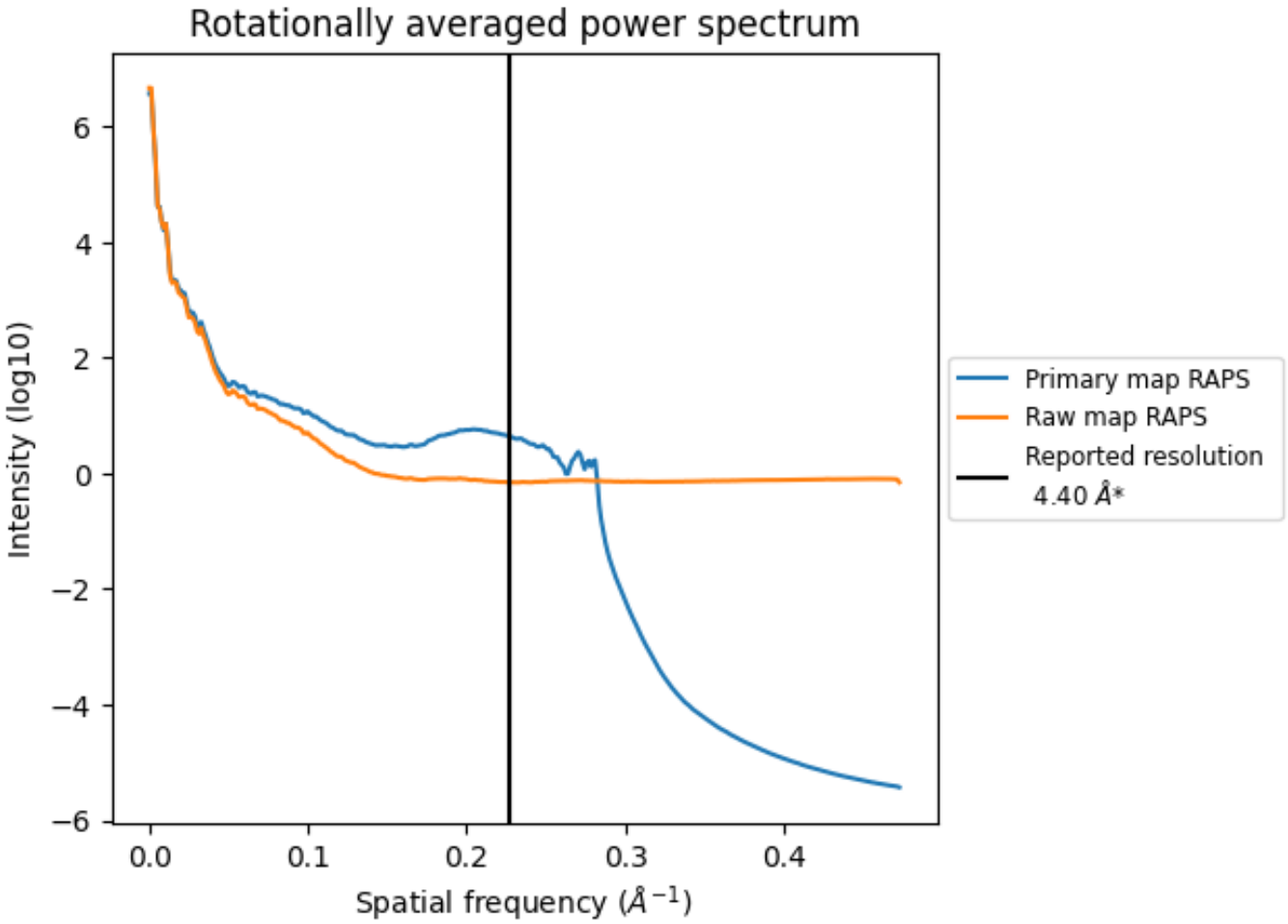
7.2 Volume estimate



The volume at the recommended contour level is 11953 nm^3; this corresponds to an approximate mass of 10798 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)

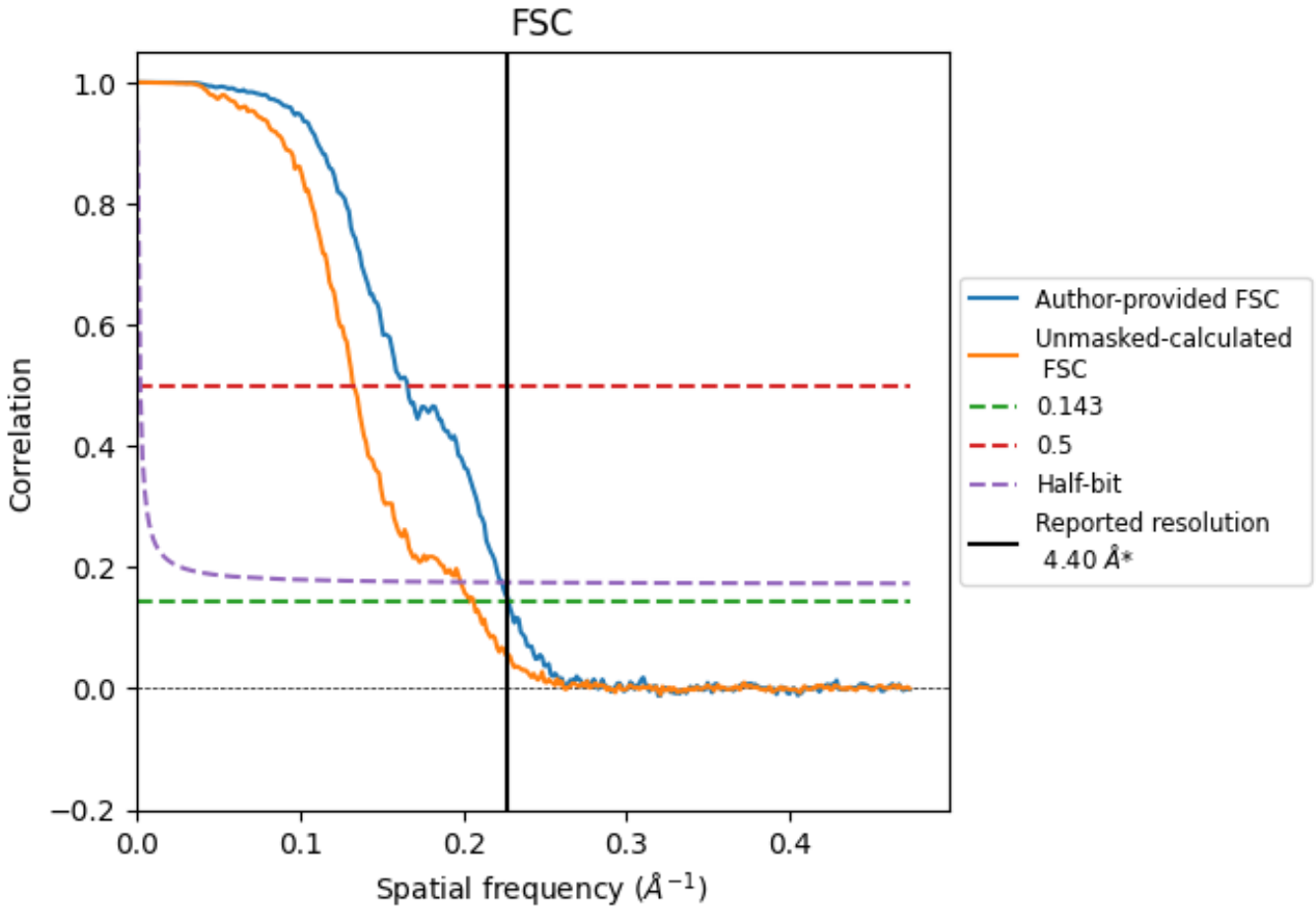


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.39	6.03	4.47
Unmasked-calculated*	4.91	7.54	5.04

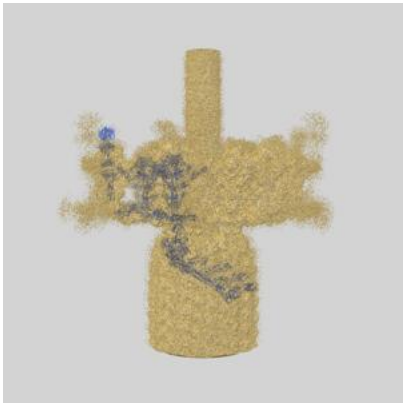
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.91 differs from the reported value 4.4 by more than 10 %

9 Map-model fit

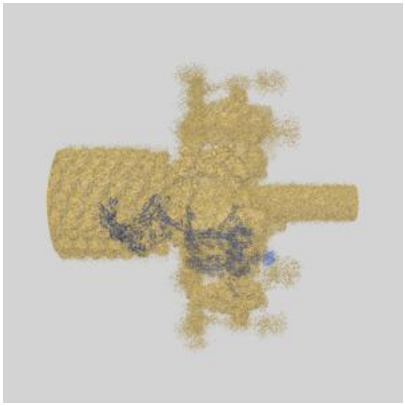
This section contains information regarding the fit between EMDB map EMD-19971 and PDB model 9EUI. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

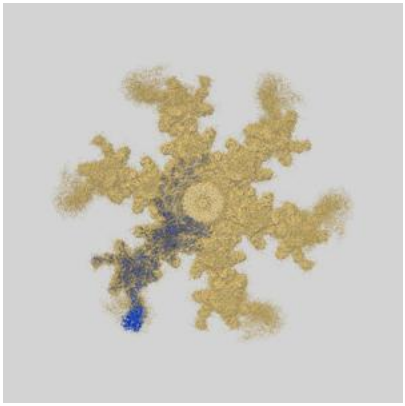
9.1.1 Map-model overlay



X

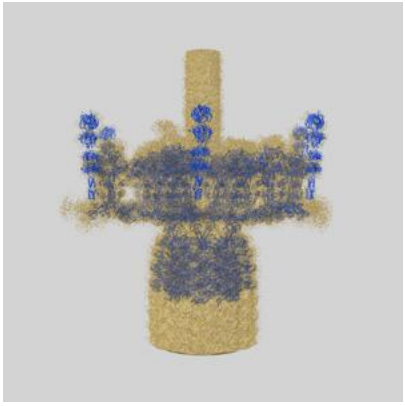


Y

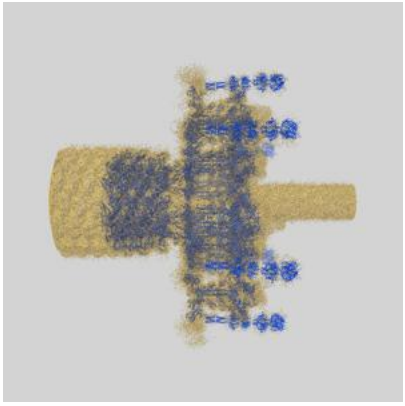


Z

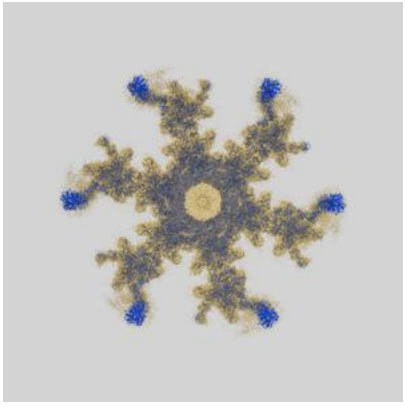
9.1.2 Map-model assembly overlay



X



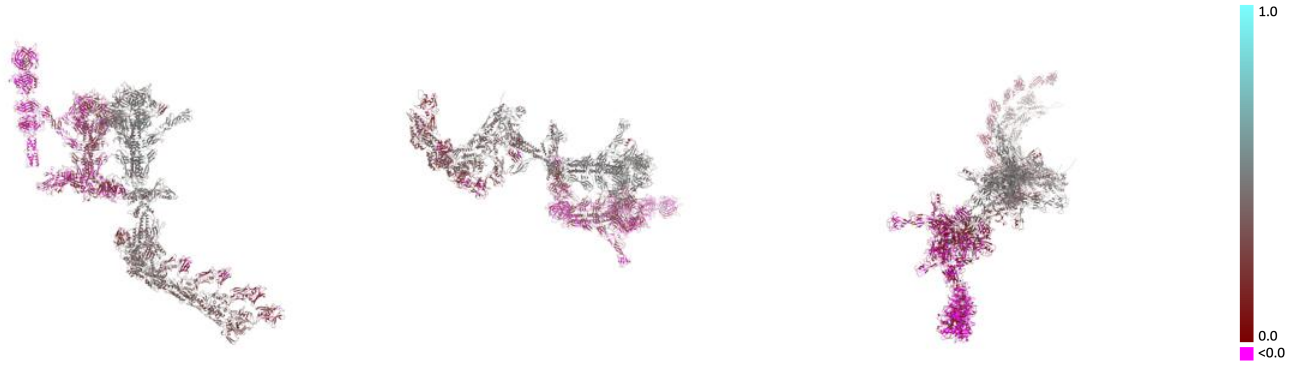
Y



Z

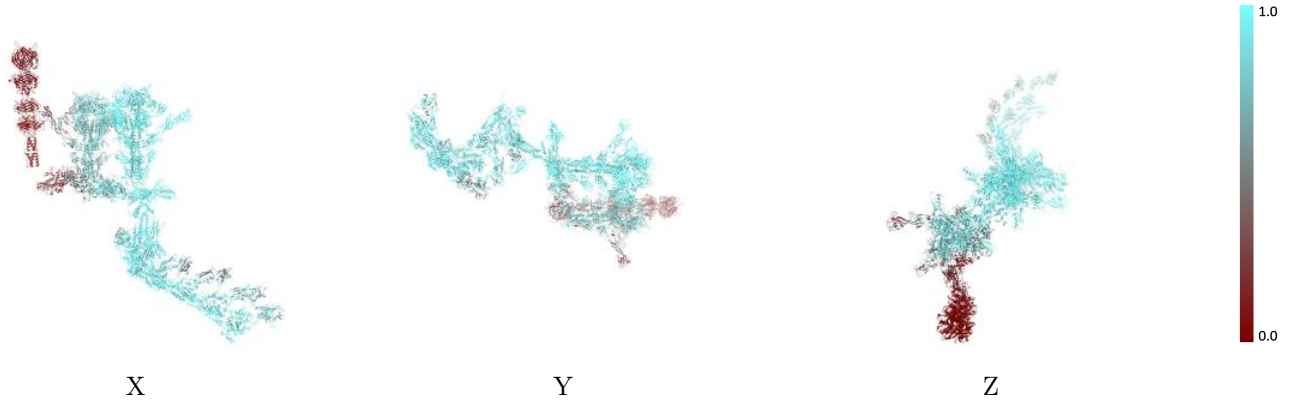
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



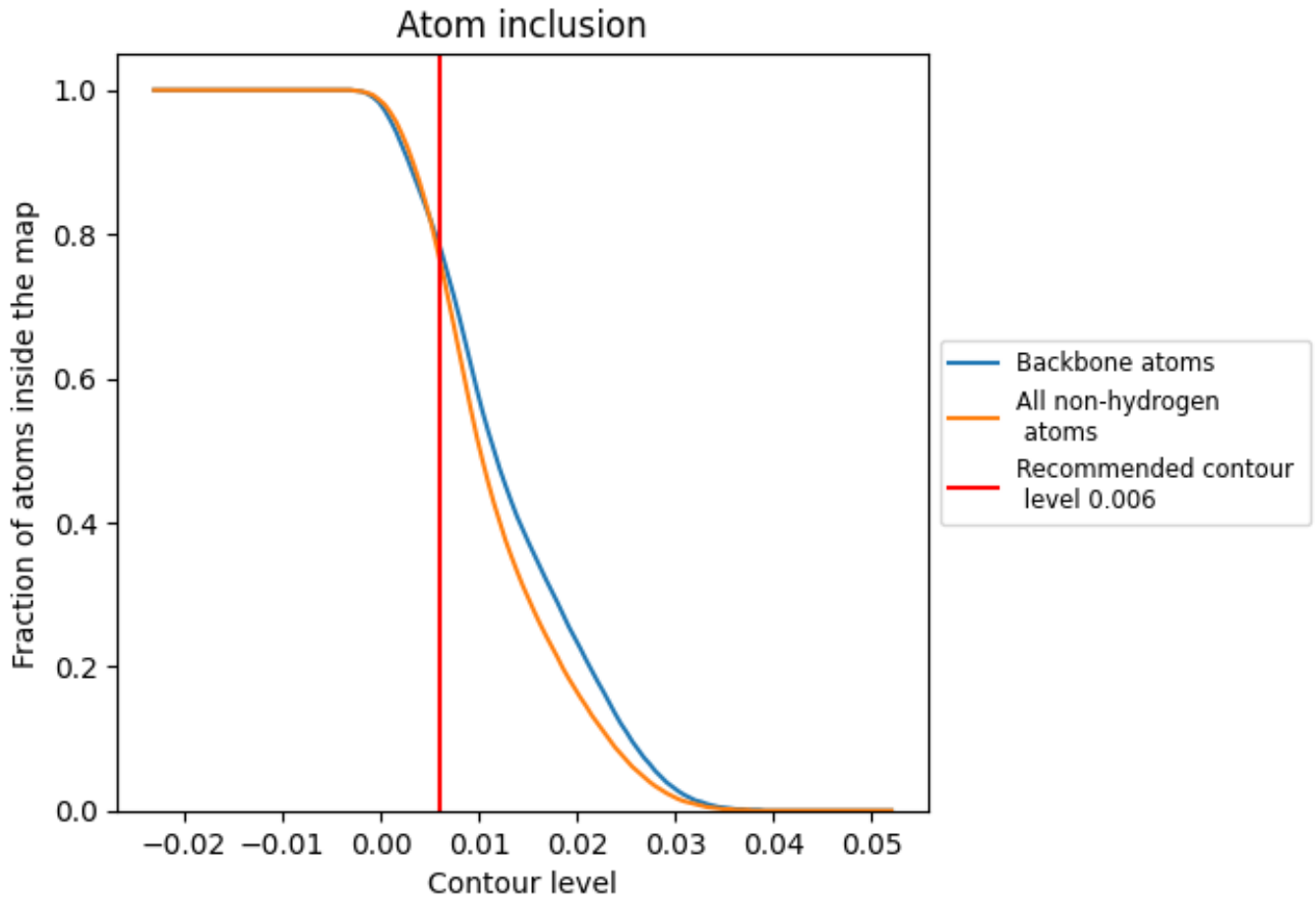
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.2730
A	0.9250	0.4230
B	0.9430	0.4230
C	0.9410	0.4210
D	0.8230	0.3060
E	0.8690	0.3620
F	0.9000	0.3670
G	0.8370	0.3160
H	0.8290	0.3100
I	0.8490	0.3010
J	0.8390	0.2860
K	0.8280	0.1420
L	0.8760	0.2240
M	0.6960	0.1560
N	0.4920	0.1130
O	0.1590	0.0760
P	0.0750	0.0540
Q	0.9440	0.4360
R	0.9430	0.4360
S	0.9440	0.4300
T	0.7550	0.1600
U	0.6990	0.1010
V	0.6770	0.1130
W	0.0250	-0.0010
X	0.0110	-0.0060
Y	0.0110	-0.0030